

FIGURE 1

## IMPDH COORDINATES

|      | Atom | Type | Residue | #  | X      | Y      | Z      | OCC  | B     |
|------|------|------|---------|----|--------|--------|--------|------|-------|
| ATOM | 1    | CB   | ALA     | 17 | 72.558 | 49.267 | 65.109 | 1.00 | 22.70 |
| ATOM | 2    | C    | ALA     | 17 | 71.313 | 51.476 | 65.238 | 1.00 | 26.93 |
| ATOM | 3    | O    | ALA     | 17 | 70.825 | 51.262 | 64.127 | 1.00 | 29.36 |
| ATOM | 4    | N    | ALA     | 17 | 71.028 | 49.819 | 66.975 | 1.00 | 26.46 |
| ATOM | 5    | CA   | ALA     | 17 | 72.022 | 50.375 | 66.030 | 1.00 | 26.18 |
| ATOM | 6    | N    | LEU     | 18 | 71.234 | 52.650 | 65.852 | 1.00 | 25.12 |
| ATOM | 7    | CA   | LEU     | 18 | 70.583 | 53.798 | 65.245 | 1.00 | 23.77 |
| ATOM | 8    | CB   | LEU     | 18 | 69.314 | 54.098 | 66.036 | 1.00 | 24.11 |
| ATOM | 9    | CG   | LEU     | 18 | 68.112 | 54.653 | 65.285 | 1.00 | 25.97 |
| ATOM | 10   | CD1  | LEU     | 18 | 67.670 | 53.647 | 64.234 | 1.00 | 20.03 |
| ATOM | 11   | CD2  | LEU     | 18 | 66.998 | 54.949 | 66.278 | 1.00 | 24.01 |
| ATOM | 12   | C    | LEU     | 18 | 71.549 | 54.973 | 65.364 | 1.00 | 22.96 |
| ATOM | 13   | O    | LEU     | 18 | 72.234 | 55.092 | 66.376 | 1.00 | 24.55 |
| ATOM | 14   | N    | THR     | 19 | 71.657 | 55.805 | 64.334 | 1.00 | 20.50 |
| ATOM | 15   | CA   | THR     | 19 | 72.555 | 56.953 | 64.418 | 1.00 | 19.77 |
| ATOM | 16   | CB   | THR     | 19 | 73.040 | 57.451 | 63.032 | 1.00 | 19.66 |
| ATOM | 17   | OG1  | THR     | 19 | 71.942 | 57.976 | 62.285 | 1.00 | 24.22 |
| ATOM | 18   | CG2  | THR     | 19 | 73.681 | 56.329 | 62.254 | 1.00 | 21.13 |
| ATOM | 19   | C    | THR     | 19 | 71.856 | 58.108 | 65.118 | 1.00 | 20.76 |
| ATOM | 20   | O    | THR     | 19 | 70.625 | 58.138 | 65.196 | 1.00 | 23.20 |
| ATOM | 21   | N    | ALA     | 20 | 72.644 | 59.064 | 65.604 | 1.00 | 20.04 |
| ATOM | 22   | CA   | ALA     | 20 | 72.129 | 60.244 | 66.286 | 1.00 | 17.52 |
| ATOM | 23   | CB   | ALA     | 20 | 73.277 | 61.136 | 66.727 | 1.00 | 16.35 |
| ATOM | 24   | C    | ALA     | 20 | 71.188 | 61.011 | 65.370 | 1.00 | 17.21 |
| ATOM | 25   | O    | ALA     | 20 | 70.121 | 61.445 | 65.789 | 1.00 | 18.45 |
| ATOM | 26   | N    | GLN     | 21 | 71.586 | 61.168 | 64.114 | 1.00 | 18.11 |
| ATOM | 27   | CA   | GLN     | 21 | 70.768 | 61.865 | 63.132 | 1.00 | 17.57 |
| ATOM | 28   | CB   | GLN     | 21 | 71.445 | 61.795 | 61.759 | 1.00 | 19.03 |
| ATOM | 29   | CG   | GLN     | 21 | 70.925 | 62.768 | 60.699 | 1.00 | 23.41 |
| ATOM | 30   | CD   | GLN     | 21 | 69.630 | 62.324 | 60.040 | 1.00 | 31.00 |
| ATOM | 31   | OE1  | GLN     | 21 | 69.245 | 61.155 | 60.105 | 1.00 | 34.26 |
| ATOM | 32   | NE2  | GLN     | 21 | 68.957 | 63.260 | 59.381 | 1.00 | 36.22 |
| ATOM | 33   | C    | GLN     | 21 | 69.383 | 61.210 | 63.093 | 1.00 | 17.94 |
| ATOM | 34   | O    | GLN     | 21 | 68.374 | 61.895 | 63.181 | 1.00 | 20.56 |
| ATOM | 35   | N    | GLN     | 22 | 69.340 | 59.883 | 63.025 | 1.00 | 15.31 |
| ATOM | 36   | CA   | GLN     | 22 | 68.072 | 59.155 | 62.976 | 1.00 | 14.95 |
| ATOM | 37   | CB   | GLN     | 22 | 68.316 | 57.682 | 62.671 | 1.00 | 14.56 |
| ATOM | 38   | CG   | GLN     | 22 | 68.906 | 57.446 | 61.307 | 1.00 | 19.65 |
| ATOM | 39   | CD   | GLN     | 22 | 69.475 | 56.058 | 61.166 | 1.00 | 28.31 |
| ATOM | 40   | OE1  | GLN     | 22 | 69.911 | 55.447 | 62.146 | 1.00 | 29.91 |
| ATOM | 41   | NE2  | GLN     | 22 | 69.499 | 55.554 | 59.939 | 1.00 | 34.86 |
| ATOM | 42   | C    | GLN     | 22 | 67.284 | 59.251 | 64.265 | 1.00 | 14.40 |
| ATOM | 43   | O    | GLN     | 22 | 66.104 | 59.559 | 64.260 | 1.00 | 17.28 |
| ATOM | 44   | N    | LEU     | 23 | 67.961 | 58.997 | 65.369 | 1.00 | 13.72 |
| ATOM | 45   | CA   | LEU     | 23 | 67.360 | 59.019 | 66.686 | 1.00 | 13.86 |
| ATOM | 46   | CB   | LEU     | 23 | 68.430 | 58.644 | 67.719 | 1.00 | 10.46 |
| ATOM | 47   | CG   | LEU     | 23 | 68.090 | 58.588 | 69.210 | 1.00 | 10.45 |
| ATOM | 48   | CD1  | LEU     | 23 | 67.222 | 57.399 | 69.478 | 1.00 | 13.28 |
| ATOM | 49   | CD2  | LEU     | 23 | 69.354 | 58.489 | 70.036 | 1.00 | 9.21  |
| ATOM | 50   | C    | LEU     | 23 | 66.698 | 60.343 | 67.072 | 1.00 | 17.33 |
| ATOM | 51   | O    | LEU     | 23 | 65.552 | 60.353 | 67.517 | 1.00 | 17.38 |
| ATOM | 52   | N    | PHE     | 24 | 67.417 | 61.454 | 66.894 | 1.00 | 22.11 |
| ATOM | 53   | CA   | PHE     | 24 | 66.926 | 62.781 | 67.282 | 1.00 | 23.93 |
| ATOM | 54   | CB   | PHE     | 24 | 68.060 | 63.626 | 67.870 | 1.00 | 18.72 |
| ATOM | 55   | CG   | PHE     | 24 | 68.688 | 63.017 | 69.084 | 1.00 | 18.19 |

FIGURE 1 (CONT.)

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 56  | CD1 | PHE | 24 | 68.056 | 63.098 | 70.321 | 1.00 | 16.51 |
| ATOM | 57  | CD2 | PHE | 24 | 69.849 | 62.270 | 68.975 | 1.00 | 16.34 |
| ATOM | 58  | CE1 | PHE | 24 | 68.573 | 62.445 | 71.422 | 1.00 | 16.81 |
| ATOM | 59  | CE2 | PHE | 24 | 70.373 | 61.614 | 70.070 | 1.00 | 17.36 |
| ATOM | 60  | CZ  | PHE | 24 | 69.732 | 61.695 | 71.295 | 1.00 | 20.29 |
| ATOM | 61  | C   | PHE | 24 | 66.228 | 63.569 | 66.212 | 1.00 | 28.47 |
| ATOM | 62  | O   | PHE | 24 | 66.123 | 64.788 | 66.308 | 1.00 | 30.83 |
| ATOM | 63  | N   | ASN | 25 | 65.728 | 62.886 | 65.197 | 1.00 | 31.66 |
| ATOM | 64  | CA  | ASN | 25 | 65.039 | 63.585 | 64.130 | 1.00 | 35.39 |
| ATOM | 65  | CB  | ASN | 25 | 65.970 | 63.788 | 62.926 | 1.00 | 37.11 |
| ATOM | 66  | CG  | ASN | 25 | 66.984 | 64.917 | 63.156 | 1.00 | 32.50 |
| ATOM | 67  | OD1 | ASN | 25 | 66.630 | 66.090 | 63.117 | 1.00 | 34.46 |
| ATOM | 68  | ND2 | ASN | 25 | 68.235 | 64.562 | 63.402 | 1.00 | 24.11 |
| ATOM | 69  | C   | ASN | 25 | 63.752 | 62.868 | 63.767 | 1.00 | 37.00 |
| ATOM | 70  | O   | ASN | 25 | 63.416 | 62.689 | 62.593 | 1.00 | 37.37 |
| ATOM | 71  | N   | CYS | 26 | 63.053 | 62.447 | 64.821 | 1.00 | 38.09 |
| ATOM | 72  | CA  | CYS | 26 | 61.768 | 61.759 | 64.725 | 1.00 | 39.40 |
| ATOM | 73  | CB  | CYS | 26 | 61.902 | 60.316 | 65.197 | 1.00 | 41.92 |
| ATOM | 74  | SG  | CYS | 26 | 63.069 | 59.371 | 64.233 | 1.00 | 54.81 |
| ATOM | 75  | C   | CYS | 26 | 60.701 | 62.474 | 65.566 | 1.00 | 39.10 |
| ATOM | 76  | O   | CYS | 26 | 59.562 | 62.020 | 65.636 | 1.00 | 40.50 |
| ATOM | 77  | N   | GLY | 27 | 61.092 | 63.563 | 66.232 | 1.00 | 37.42 |
| ATOM | 78  | CA  | GLY | 27 | 60.169 | 64.345 | 67.044 | 1.00 | 34.99 |
| ATOM | 79  | C   | GLY | 27 | 59.622 | 63.721 | 68.319 | 1.00 | 33.08 |
| ATOM | 80  | O   | GLY | 27 | 58.602 | 64.171 | 68.843 | 1.00 | 33.66 |
| ATOM | 81  | N   | ASP | 28 | 60.324 | 62.731 | 68.857 | 1.00 | 29.48 |
| ATOM | 82  | CA  | ASP | 28 | 59.872 | 62.053 | 70.061 | 1.00 | 26.13 |
| ATOM | 83  | CB  | ASP | 28 | 60.518 | 60.669 | 70.156 | 1.00 | 31.57 |
| ATOM | 84  | CG  | ASP | 28 | 60.062 | 59.717 | 69.058 | 1.00 | 37.50 |
| ATOM | 85  | OD1 | ASP | 28 | 59.113 | 60.055 | 68.313 | 1.00 | 42.70 |
| ATOM | 86  | OD2 | ASP | 28 | 60.651 | 58.615 | 68.949 | 1.00 | 40.12 |
| ATOM | 87  | C   | ASP | 28 | 60.107 | 62.803 | 71.368 | 1.00 | 24.31 |
| ATOM | 88  | O   | ASP | 28 | 59.607 | 62.382 | 72.405 | 1.00 | 26.33 |
| ATOM | 89  | N   | GLY | 29 | 60.879 | 63.885 | 71.340 | 1.00 | 20.96 |
| ATOM | 90  | CA  | GLY | 29 | 61.152 | 64.622 | 72.564 | 1.00 | 17.97 |
| ATOM | 91  | C   | GLY | 29 | 61.908 | 63.793 | 73.597 | 1.00 | 19.01 |
| ATOM | 92  | O   | GLY | 29 | 61.468 | 63.660 | 74.748 | 1.00 | 21.20 |
| ATOM | 93  | N   | LEU | 30 | 63.065 | 63.261 | 73.197 | 1.00 | 17.09 |
| ATOM | 94  | CA  | LEU | 30 | 63.892 | 62.416 | 74.057 | 1.00 | 12.60 |
| ATOM | 95  | CB  | LEU | 30 | 64.817 | 61.547 | 73.212 | 1.00 | 9.93  |
| ATOM | 96  | CG  | LEU | 30 | 64.233 | 60.723 | 72.068 | 1.00 | 10.94 |
| ATOM | 97  | CD1 | LEU | 30 | 65.388 | 60.127 | 71.284 | 1.00 | 9.88  |
| ATOM | 98  | CD2 | LEU | 30 | 63.302 | 59.628 | 72.598 | 1.00 | 11.80 |
| ATOM | 99  | C   | LEU | 30 | 64.762 | 63.194 | 75.021 | 1.00 | 13.15 |
| ATOM | 100 | O   | LEU | 30 | 65.039 | 64.376 | 74.824 | 1.00 | 12.25 |
| ATOM | 101 | N   | THR | 31 | 65.290 | 62.474 | 75.998 | 1.00 | 12.92 |
| ATOM | 102 | CA  | THR | 31 | 66.164 | 63.037 | 77.006 | 1.00 | 16.46 |
| ATOM | 103 | CB  | THR | 31 | 65.392 | 63.352 | 78.279 | 1.00 | 22.29 |
| ATOM | 104 | OG1 | THR | 31 | 64.263 | 64.164 | 77.961 | 1.00 | 33.50 |
| ATOM | 105 | CG2 | THR | 31 | 66.253 | 64.121 | 79.219 | 1.00 | 25.29 |
| ATOM | 106 | C   | THR | 31 | 67.204 | 61.969 | 77.318 | 1.00 | 16.75 |
| ATOM | 107 | O   | THR | 31 | 67.076 | 60.831 | 76.863 | 1.00 | 18.24 |
| ATOM | 108 | N   | TYR | 32 | 68.207 | 62.328 | 78.113 | 1.00 | 14.54 |
| ATOM | 109 | CA  | TYR | 32 | 69.281 | 61.418 | 78.493 | 1.00 | 13.73 |
| ATOM | 110 | CB  | TYR | 32 | 70.114 | 62.029 | 79.623 | 1.00 | 14.15 |
| ATOM | 111 | CG  | TYR | 32 | 70.778 | 63.348 | 79.275 | 1.00 | 13.25 |
| ATOM | 112 | CD1 | TYR | 32 | 71.485 | 63.498 | 78.087 | 1.00 | 11.60 |
| ATOM | 113 | CE1 | TYR | 32 | 72.102 | 64.696 | 77.770 | 1.00 | 11.18 |

FIGURE 1 (CONT.)

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 114 | CD2 | TYR | 32 | 70.708 | 64.443 | 80.143 | 1.00 | 9.67  |
| ATOM | 115 | CE2 | TYR | 32 | 71.323 | 65.641 | 79.831 | 1.00 | 5.87  |
| ATOM | 116 | CZ  | TYR | 32 | 72.020 | 65.759 | 78.645 | 1.00 | 9.04  |
| ATOM | 117 | OH  | TYR | 32 | 72.646 | 66.936 | 78.322 | 1.00 | 12.17 |
| ATOM | 118 | C   | TYR | 32 | 68.836 | 60.014 | 78.895 | 1.00 | 14.12 |
| ATOM | 119 | O   | TYR | 32 | 69.377 | 59.028 | 78.412 | 1.00 | 15.71 |
| ATOM | 120 | N   | ASN | 33 | 67.844 | 59.919 | 79.770 | 1.00 | 13.11 |
| ATOM | 121 | CA  | ASN | 33 | 67.371 | 58.614 | 80.217 | 1.00 | 11.54 |
| ATOM | 122 | CB  | ASN | 33 | 66.496 | 58.768 | 81.462 | 1.00 | 11.83 |
| ATOM | 123 | CG  | ASN | 33 | 67.311 | 59.056 | 82.713 | 1.00 | 17.66 |
| ATOM | 124 | OD1 | ASN | 33 | 68.541 | 59.127 | 82.665 | 1.00 | 23.03 |
| ATOM | 125 | ND2 | ASN | 33 | 66.634 | 59.216 | 83.840 | 1.00 | 20.22 |
| ATOM | 126 | C   | ASN | 33 | 66.628 | 57.803 | 79.162 | 1.00 | 9.67  |
| ATOM | 127 | O   | ASN | 33 | 66.382 | 56.632 | 79.359 | 1.00 | 11.34 |
| ATOM | 128 | N   | ASP | 34 | 66.314 | 58.411 | 78.027 | 1.00 | 10.31 |
| ATOM | 129 | CA  | ASP | 34 | 65.565 | 57.730 | 76.980 | 1.00 | 9.62  |
| ATOM | 130 | CB  | ASP | 34 | 64.693 | 58.723 | 76.202 | 1.00 | 7.60  |
| ATOM | 131 | CG  | ASP | 34 | 63.702 | 59.452 | 77.080 | 1.00 | 10.75 |
| ATOM | 132 | OD1 | ASP | 34 | 62.884 | 58.790 | 77.743 | 1.00 | 16.59 |
| ATOM | 133 | OD2 | ASP | 34 | 63.728 | 60.695 | 77.105 | 1.00 | 16.20 |
| ATOM | 134 | C   | ASP | 34 | 66.410 | 56.951 | 75.996 | 1.00 | 10.82 |
| ATOM | 135 | O   | ASP | 34 | 65.857 | 56.330 | 75.088 | 1.00 | 12.67 |
| ATOM | 136 | N   | PHE | 35 | 67.732 | 56.997 | 76.119 | 1.00 | 10.03 |
| ATOM | 137 | CA  | PHE | 35 | 68.566 | 56.251 | 75.180 | 1.00 | 11.20 |
| ATOM | 138 | CB  | PHE | 35 | 68.809 | 57.065 | 73.905 | 1.00 | 8.60  |
| ATOM | 139 | CG  | PHE | 35 | 69.723 | 58.235 | 74.093 | 1.00 | 5.90  |
| ATOM | 140 | CD1 | PHE | 35 | 69.222 | 59.467 | 74.457 | 1.00 | 2.20  |
| ATOM | 141 | CD2 | PHE | 35 | 71.095 | 58.094 | 73.916 | 1.00 | 9.58  |
| ATOM | 142 | CE1 | PHE | 35 | 70.059 | 60.547 | 74.628 | 1.00 | 5.47  |
| ATOM | 143 | CE2 | PHE | 35 | 71.944 | 59.166 | 74.085 | 1.00 | 8.35  |
| ATOM | 144 | CZ  | PHE | 35 | 71.423 | 60.399 | 74.450 | 1.00 | 10.50 |
| ATOM | 145 | C   | PHE | 35 | 69.892 | 55.758 | 75.748 | 1.00 | 12.61 |
| ATOM | 146 | O   | PHE | 35 | 70.284 | 56.119 | 76.859 | 1.00 | 13.92 |
| ATOM | 147 | N   | LEU | 36 | 70.568 | 54.917 | 74.972 | 1.00 | 14.59 |
| ATOM | 148 | CA  | LEU | 36 | 71.863 | 54.348 | 75.346 | 1.00 | 14.60 |
| ATOM | 149 | CB  | LEU | 36 | 71.712 | 52.852 | 75.647 | 1.00 | 15.42 |
| ATOM | 150 | CG  | LEU | 36 | 71.050 | 52.471 | 76.958 | 1.00 | 15.98 |
| ATOM | 151 | CD1 | LEU | 36 | 70.772 | 50.996 | 76.982 | 1.00 | 12.63 |
| ATOM | 152 | CD2 | LEU | 36 | 71.943 | 52.880 | 78.105 | 1.00 | 19.66 |
| ATOM | 153 | C   | LEU | 36 | 72.825 | 54.475 | 74.183 | 1.00 | 13.79 |
| ATOM | 154 | O   | LEU | 36 | 72.402 | 54.693 | 73.046 | 1.00 | 15.53 |
| ATOM | 155 | N   | ILE | 37 | 74.117 | 54.370 | 74.468 | 1.00 | 13.37 |
| ATOM | 156 | CA  | ILE | 37 | 75.114 | 54.398 | 73.412 | 1.00 | 11.78 |
| ATOM | 157 | CB  | ILE | 37 | 76.301 | 55.330 | 73.708 | 1.00 | 12.62 |
| ATOM | 158 | CG2 | ILE | 37 | 77.117 | 55.521 | 72.432 | 1.00 | 9.76  |
| ATOM | 159 | CG1 | ILE | 37 | 75.818 | 56.695 | 74.204 | 1.00 | 9.90  |
| ATOM | 160 | CD1 | ILE | 37 | 76.942 | 57.594 | 74.695 | 1.00 | 3.11  |
| ATOM | 161 | C   | ILE | 37 | 75.616 | 52.963 | 73.403 | 1.00 | 11.63 |
| ATOM | 162 | O   | ILE | 37 | 75.927 | 52.406 | 74.464 | 1.00 | 9.34  |
| ATOM | 163 | N   | LEU | 38 | 75.605 | 52.347 | 72.225 | 1.00 | 12.19 |
| ATOM | 164 | CA  | LEU | 38 | 76.048 | 50.964 | 72.067 | 1.00 | 12.98 |
| ATOM | 165 | CB  | LEU | 38 | 75.474 | 50.372 | 70.778 | 1.00 | 12.87 |
| ATOM | 166 | CG  | LEU | 38 | 74.129 | 49.627 | 70.830 | 1.00 | 9.25  |
| ATOM | 167 | CD1 | LEU | 38 | 73.238 | 50.120 | 71.943 | 1.00 | 7.47  |
| ATOM | 168 | CD2 | LEU | 38 | 73.445 | 49.763 | 69.494 | 1.00 | 3.33  |
| ATOM | 169 | C   | LEU | 38 | 77.572 | 50.880 | 72.067 | 1.00 | 16.00 |
| ATOM | 170 | O   | LEU | 38 | 78.244 | 51.672 | 71.402 | 1.00 | 18.83 |
| ATOM | 171 | N   | PRO | 39 | 78.134 | 49.894 | 72.803 | 1.00 | 14.92 |

FIGURE 1 (CONT.)

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 172 | CD  | PRO | 39 | 77.416 | 48.835 | 73.528 | 1.00 | 16.09 |
| ATOM | 173 | CA  | PRO | 39 | 79.578 | 49.702 | 72.899 | 1.00 | 14.01 |
| ATOM | 174 | CB  | PRO | 39 | 79.688 | 48.579 | 73.928 | 1.00 | 14.77 |
| ATOM | 175 | CG  | PRO | 39 | 78.470 | 47.778 | 73.672 | 1.00 | 16.81 |
| ATOM | 176 | C   | PRO | 39 | 80.247 | 49.339 | 71.574 | 1.00 | 15.63 |
| ATOM | 177 | O   | PRO | 39 | 79.639 | 48.687 | 70.713 | 1.00 | 15.28 |
| ATOM | 178 | N   | GLY | 40 | 81.513 | 49.736 | 71.439 | 1.00 | 14.98 |
| ATOM | 179 | CA  | GLY | 40 | 82.262 | 49.470 | 70.230 | 1.00 | 12.21 |
| ATOM | 180 | C   | GLY | 40 | 83.409 | 48.495 | 70.399 | 1.00 | 13.01 |
| ATOM | 181 | O   | GLY | 40 | 83.224 | 47.389 | 70.919 | 1.00 | 12.38 |
| ATOM | 182 | N   | TYR | 41 | 84.583 | 48.892 | 69.904 | 1.00 | 13.42 |
| ATOM | 183 | CA  | TYR | 41 | 65.794 | 48.077 | 69.957 | 1.00 | 13.37 |
| ATOM | 184 | CB  | TYR | 41 | 86.353 | 47.862 | 68.551 | 1.00 | 13.51 |
| ATOM | 185 | CG  | TYR | 41 | 87.638 | 47.069 | 68.546 | 1.00 | 21.45 |
| ATOM | 186 | CD1 | TYR | 41 | 87.680 | 45.770 | 69.050 | 1.00 | 24.36 |
| ATOM | 187 | CE1 | TYR | 41 | 88.863 | 45.046 | 69.069 | 1.00 | 28.32 |
| ATOM | 188 | CD2 | TYR | 41 | 88.818 | 47.625 | 68.064 | 1.00 | 26.04 |
| ATOM | 189 | CE2 | TYR | 41 | 90.013 | 46.910 | 68.082 | 1.00 | 25.88 |
| ATOM | 190 | CZ  | TYR | 41 | 90.029 | 45.623 | 68.585 | 1.00 | 27.54 |
| ATOM | 191 | OH  | TYR | 41 | 91.211 | 44.917 | 68.607 | 1.00 | 29.43 |
| ATOM | 192 | C   | TYR | 41 | 86.861 | 48.731 | 70.824 | 1.00 | 14.08 |
| ATOM | 193 | O   | TYR | 41 | 87.248 | 49.878 | 70.588 | 1.00 | 14.99 |
| ATOM | 194 | N   | ILE | 42 | 87.381 | 47.980 | 71.785 | 1.00 | 14.83 |
| ATOM | 195 | CA  | ILE | 42 | 88.390 | 48.518 | 72.691 | 1.00 | 16.98 |
| ATOM | 196 | CB  | ILE | 42 | 88.076 | 48.131 | 74.151 | 1.00 | 17.07 |
| ATOM | 197 | CG2 | ILE | 42 | 89.107 | 48.739 | 75.098 | 1.00 | 14.32 |
| ATOM | 198 | CG1 | ILE | 42 | 86.650 | 48.568 | 74.507 | 1.00 | 16.63 |
| ATOM | 199 | CD1 | ILE | 42 | 86.157 | 48.016 | 75.818 | 1.00 | 15.82 |
| ATOM | 200 | C   | ILE | 42 | 89.795 | 48.048 | 72.352 | 1.00 | 18.11 |
| ATOM | 201 | O   | ILE | 42 | 90.060 | 46.844 | 72.285 | 1.00 | 19.16 |
| ATOM | 202 | N   | ASP | 43 | 90.692 | 49.000 | 72.129 | 1.00 | 17.76 |
| ATOM | 203 | CA  | ASP | 43 | 92.082 | 48.683 | 71.826 | 1.00 | 20.06 |
| ATOM | 204 | CB  | ASP | 43 | 92.331 | 48.676 | 70.312 | 1.00 | 20.24 |
| ATOM | 205 | CG  | ASP | 43 | 92.245 | 50.056 | 69.682 | 1.00 | 23.30 |
| ATOM | 206 | OD1 | ASP | 43 | 91.509 | 50.936 | 70.186 | 1.00 | 23.90 |
| ATOM | 207 | OD2 | ASP | 43 | 92.915 | 50.248 | 68.648 | 1.00 | 25.65 |
| ATOM | 208 | C   | ASP | 43 | 93.016 | 49.659 | 72.540 | 1.00 | 20.53 |
| ATOM | 209 | O   | ASP | 43 | 94.110 | 49.955 | 72.071 | 1.00 | 21.86 |
| ATOM | 210 | N   | PHE | 44 | 92.564 | 50.152 | 73.685 | 1.00 | 19.12 |
| ATOM | 211 | CA  | PHE | 44 | 93.323 | 51.091 | 74.488 | 1.00 | 19.11 |
| ATOM | 212 | CB  | PHE | 44 | 93.219 | 52.509 | 73.910 | 1.00 | 22.06 |
| ATOM | 213 | CG  | PHE | 44 | 91.816 | 53.051 | 73.883 | 1.00 | 26.32 |
| ATOM | 214 | CD1 | PHE | 44 | 90.925 | 52.675 | 72.871 | 1.00 | 23.08 |
| ATOM | 215 | CD2 | PHE | 44 | 91.367 | 53.904 | 74.890 | 1.00 | 26.77 |
| ATOM | 216 | CE1 | PHE | 44 | 89.612 | 53.131 | 72.866 | 1.00 | 19.60 |
| ATOM | 217 | CE2 | PHE | 44 | 90.053 | 54.363 | 74.893 | 1.00 | 27.23 |
| ATOM | 218 | CZ  | PHE | 44 | 89.174 | 53.974 | 73.875 | 1.00 | 23.92 |
| ATOM | 219 | C   | PHE | 44 | 92.716 | 51.039 | 75.881 | 1.00 | 19.64 |
| ATOM | 220 | O   | PHE | 44 | 91.666 | 50.418 | 76.085 | 1.00 | 19.73 |
| ATOM | 221 | N   | THR | 45 | 93.359 | 51.699 | 76.834 | 1.00 | 19.57 |
| ATOM | 222 | CA  | THR | 45 | 92.871 | 51.699 | 78.203 | 1.00 | 20.17 |
| ATOM | 223 | CB  | THR | 45 | 94.015 | 51.487 | 79.185 | 1.00 | 21.18 |
| ATOM | 224 | OG1 | THR | 45 | 95.014 | 52.488 | 78.966 | 1.00 | 25.33 |
| ATOM | 225 | CG2 | THR | 45 | 94.623 | 50.113 | 78.988 | 1.00 | 18.41 |
| ATOM | 226 | C   | THR | 45 | 92.144 | 52.985 | 78.560 | 1.00 | 18.54 |
| ATOM | 227 | O   | THR | 45 | 92.360 | 54.024 | 77.944 | 1.00 | 18.57 |
| ATOM | 228 | N   | ALA | 46 | 91.310 | 52.914 | 79.589 | 1.00 | 17.69 |
| ATOM | 229 | CA  | ALA | 46 | 90.541 | 54.066 | 80.030 | 1.00 | 17.75 |

FIGURE 1 (CONT.)

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 230 | CB  | ALA | 46 | 89.709 | 53.719 | 81.253 | 1.00 | 13.85 |
| ATOM | 231 | C   | ALA | 46 | 91.441 | 55.251 | 80.315 | 1.00 | 18.75 |
| ATOM | 232 | O   | ALA | 46 | 91.138 | 56.367 | 79.917 | 1.00 | 20.63 |
| ATOM | 233 | N   | ASP | 47 | 92.582 | 55.001 | 80.944 | 1.00 | 20.24 |
| ATOM | 234 | CA  | ASP | 47 | 93.504 | 56.088 | 81.268 | 1.00 | 21.37 |
| ATOM | 235 | CB  | ASP | 47 | 94.580 | 55.645 | 82.278 | 1.00 | 25.83 |
| ATOM | 236 | CG  | ASP | 47 | 95.352 | 54.403 | 81.837 | 1.00 | 35.96 |
| ATOM | 237 | OD1 | ASP | 47 | 96.462 | 54.556 | 81.274 | 1.00 | 38.06 |
| ATOM | 238 | OD2 | ASP | 47 | 94.870 | 53.269 | 82.091 | 1.00 | 42.93 |
| ATOM | 239 | C   | ASP | 47 | 94.129 | 56.778 | 80.060 | 1.00 | 19.38 |
| ATOM | 240 | O   | ASP | 47 | 94.754 | 57.822 | 80.196 | 1.00 | 19.83 |
| ATOM | 241 | N   | GLN | 48 | 93.920 | 56.222 | 78.874 | 1.00 | 18.14 |
| ATOM | 242 | CA  | GLN | 48 | 94.477 | 56.808 | 77.665 | 1.00 | 18.72 |
| ATOM | 243 | CB  | GLN | 48 | 94.867 | 55.713 | 76.667 | 1.00 | 20.43 |
| ATOM | 244 | CG  | GLN | 48 | 96.117 | 54.922 | 77.038 | 1.00 | 25.96 |
| ATOM | 245 | CD  | GLN | 48 | 96.606 | 54.032 | 75.900 | 1.00 | 31.16 |
| ATOM | 246 | OE1 | GLN | 48 | 97.052 | 54.519 | 74.857 | 1.00 | 30.37 |
| ATOM | 247 | NE2 | GLN | 48 | 96.520 | 52.721 | 76.096 | 1.00 | 33.58 |
| ATOM | 248 | C   | GLN | 48 | 93.510 | 57.772 | 77.000 | 1.00 | 20.23 |
| ATOM | 249 | O   | GLN | 48 | 93.840 | 58.387 | 75.985 | 1.00 | 22.71 |
| ATOM | 250 | N   | VAL | 49 | 92.311 | 57.896 | 77.558 | 1.00 | 20.36 |
| ATOM | 251 | CA  | VAL | 49 | 91.286 | 58.771 | 76.997 | 1.00 | 18.46 |
| ATOM | 252 | CB  | VAL | 49 | 89.878 | 58.347 | 77.489 | 1.00 | 19.19 |
| ATOM | 253 | CG1 | VAL | 49 | 88.826 | 59.354 | 77.039 | 1.00 | 22.83 |
| ATOM | 254 | CG2 | VAL | 49 | 89.545 | 56.957 | 76.964 | 1.00 | 17.01 |
| ATOM | 255 | C   | VAL | 49 | 91.540 | 60.240 | 77.315 | 1.00 | 15.71 |
| ATOM | 256 | O   | VAL | 49 | 91.771 | 60.601 | 78.465 | 1.00 | 16.81 |
| ATOM | 257 | N   | ASP | 50 | 91.482 | 61.083 | 76.291 | 1.00 | 14.39 |
| ATOM | 258 | CA  | ASP | 50 | 91.711 | 62.514 | 76.455 | 1.00 | 14.04 |
| ATOM | 259 | CB  | ASP | 50 | 92.620 | 63.027 | 75.338 | 1.00 | 11.59 |
| ATOM | 260 | CG  | ASP | 50 | 92.982 | 64.500 | 75.497 | 1.00 | 15.45 |
| ATOM | 261 | OD1 | ASP | 50 | 93.099 | 65.001 | 76.641 | 1.00 | 19.60 |
| ATOM | 262 | OD2 | ASP | 50 | 93.166 | 65.160 | 74.460 | 1.00 | 18.29 |
| ATOM | 263 | C   | ASP | 50 | 90.396 | 63.299 | 76.466 | 1.00 | 13.17 |
| ATOM | 264 | O   | ASP | 50 | 89.600 | 63.207 | 75.529 | 1.00 | 14.97 |
| ATOM | 265 | N   | LEU | 51 | 90.199 | 64.101 | 77.508 | 1.00 | 11.28 |
| ATOM | 266 | CA  | LEU | 51 | 88.989 | 64.899 | 77.658 | 1.00 | 10.04 |
| ATOM | 267 | CB  | LEU | 51 | 88.452 | 64.770 | 79.080 | 1.00 | 8.54  |
| ATOM | 268 | CG  | LEU | 51 | 88.308 | 63.399 | 79.734 | 1.00 | 5.22  |
| ATOM | 269 | CD1 | LEU | 51 | 87.731 | 63.609 | 81.122 | 1.00 | 3.10  |
| ATOM | 270 | CD2 | LEU | 51 | 87.404 | 62.485 | 78.912 | 1.00 | 8.97  |
| ATOM | 271 | C   | LEU | 51 | 89.153 | 66.390 | 77.337 | 1.00 | 10.78 |
| ATOM | 272 | O   | LEU | 51 | 88.289 | 67.187 | 77.688 | 1.00 | 12.28 |
| ATOM | 273 | N   | THR | 52 | 90.247 | 66.776 | 76.688 | 1.00 | 12.96 |
| ATOM | 274 | CA  | THR | 52 | 90.476 | 68.181 | 76.347 | 1.00 | 12.08 |
| ATOM | 275 | CB  | THR | 52 | 91.721 | 68.340 | 75.469 | 1.00 | 12.55 |
| ATOM | 276 | OG1 | THR | 52 | 92.867 | 67.868 | 76.191 | 1.00 | 10.40 |
| ATOM | 277 | CG2 | THR | 52 | 91.930 | 69.795 | 75.090 | 1.00 | 15.12 |
| ATOM | 278 | C   | THR | 52 | 89.254 | 68.722 | 75.627 | 1.00 | 11.99 |
| ATOM | 279 | O   | THR | 52 | 88.798 | 68.142 | 74.644 | 1.00 | 13.13 |
| ATOM | 280 | N   | SER | 53 | 88.731 | 69.837 | 76.120 | 1.00 | 11.60 |
| ATOM | 281 | CA  | SER | 53 | 87.530 | 70.412 | 75.548 | 1.00 | 11.26 |
| ATOM | 282 | CB  | SER | 53 | 86.325 | 69.983 | 76.377 | 1.00 | 13.37 |
| ATOM | 283 | OG  | SER | 53 | 86.159 | 68.577 | 76.326 | 1.00 | 17.69 |
| ATOM | 284 | C   | SER | 53 | 87.554 | 71.922 | 75.445 | 1.00 | 11.98 |
| ATOM | 285 | O   | SER | 53 | 88.144 | 72.607 | 76.276 | 1.00 | 13.12 |
| ATOM | 286 | N   | ALA | 54 | 86.894 | 72.435 | 74.416 | 1.00 | 11.95 |
| ATOM | 287 | CA  | ALA | 54 | 86.817 | 73.864 | 74.173 | 1.00 | 12.45 |

FIGURE 1 (CONT.)

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 288 | CB  | ALA | 54 | 86.566 | 74.122 | 72.693 | 1.00 | 8.03  |
| ATOM | 289 | C   | ALA | 54 | 85.699 | 74.486 | 74.997 | 1.00 | 15.40 |
| ATOM | 290 | O   | ALA | 54 | 84.527 | 74.138 | 74.821 | 1.00 | 17.45 |
| ATOM | 291 | N   | LEU | 55 | 86.056 | 75.371 | 75.920 | 1.00 | 15.11 |
| ATOM | 292 | CA  | LEU | 55 | 85.052 | 76.052 | 76.722 | 1.00 | 15.35 |
| ATOM | 293 | CB  | LEU | 55 | 85.679 | 76.793 | 77.905 | 1.00 | 11.75 |
| ATOM | 294 | CG  | LEU | 55 | 84.652 | 77.545 | 78.753 | 1.00 | 5.59  |
| ATOM | 295 | CD1 | LEU | 55 | 83.821 | 76.562 | 79.548 | 1.00 | 2.00  |
| ATOM | 296 | CD2 | LEU | 55 | 85.338 | 78.506 | 79.685 | 1.00 | 7.88  |
| ATOM | 297 | C   | LEU | 55 | 84.398 | 77.062 | 75.795 | 1.00 | 16.99 |
| ATOM | 298 | O   | LEU | 55 | 83.183 | 77.132 | 75.703 | 1.00 | 19.02 |
| ATOM | 299 | N   | THR | 56 | 85.216 | 77.843 | 75.102 | 1.00 | 17.95 |
| ATOM | 300 | CA  | THR | 56 | 84.707 | 78.844 | 74.179 | 1.00 | 18.88 |
| ATOM | 301 | CB  | THR | 56 | 84.709 | 80.275 | 74.804 | 1.00 | 16.13 |
| ATOM | 302 | OG1 | THR | 56 | 86.054 | 80.712 | 75.017 | 1.00 | 14.10 |
| ATOM | 303 | CG2 | THR | 56 | 83.970 | 80.300 | 76.145 | 1.00 | 16.08 |
| ATOM | 304 | C   | THR | 56 | 85.614 | 78.815 | 72.955 | 1.00 | 20.87 |
| ATOM | 305 | O   | THR | 56 | 86.517 | 77.980 | 72.869 | 1.00 | 23.00 |
| ATOM | 306 | N   | LYS | 57 | 85.371 | 79.718 | 72.011 | 1.00 | 21.01 |
| ATOM | 307 | CA  | LYS | 57 | 86.174 | 79.799 | 70.805 | 1.00 | 20.04 |
| ATOM | 308 | CB  | LYS | 57 | 85.741 | 80.986 | 69.955 | 1.00 | 18.70 |
| ATOM | 309 | CG  | LYS | 57 | 84.745 | 80.615 | 68.891 | 1.00 | 21.51 |
| ATOM | 310 | CD  | LYS | 57 | 84.338 | 81.805 | 68.056 | 1.00 | 23.91 |
| ATOM | 311 | CE  | LYS | 57 | 83.449 | 81.350 | 66.915 | 1.00 | 32.96 |
| ATOM | 312 | NZ  | LYS | 57 | 82.765 | 82.469 | 66.212 | 1.00 | 36.85 |
| ATOM | 313 | C   | LYS | 57 | 87.661 | 79.894 | 71.089 | 1.00 | 22.00 |
| ATOM | 314 | O   | LYS | 57 | 88.469 | 79.549 | 70.238 | 1.00 | 25.73 |
| ATOM | 315 | N   | LYS | 58 | 88.033 | 80.380 | 72.267 | 1.00 | 22.39 |
| ATOM | 316 | CA  | LYS | 58 | 89.444 | 80.490 | 72.598 | 1.00 | 23.85 |
| ATOM | 317 | CB  | LYS | 58 | 89.927 | 81.933 | 72.445 | 1.00 | 25.83 |
| ATOM | 318 | CG  | LYS | 58 | 89.896 | 82.442 | 71.001 | 1.00 | 28.99 |
| ATOM | 319 | CD  | LYS | 58 | 90.874 | 83.590 | 70.769 | 1.00 | 34.75 |
| ATOM | 320 | CE  | LYS | 58 | 90.656 | 84.733 | 71.755 | 1.00 | 42.57 |
| ATOM | 321 | NZ  | LYS | 58 | 91.646 | 85.843 | 71.599 | 1.00 | 44.82 |
| ATOM | 322 | C   | LYS | 58 | 89.847 | 79.921 | 73.958 | 1.00 | 25.84 |
| ATOM | 323 | O   | LYS | 58 | 91.034 | 79.809 | 74.240 | 1.00 | 28.83 |
| ATOM | 324 | N   | ILE | 59 | 88.882 | 79.596 | 74.817 | 1.00 | 24.95 |
| ATOM | 325 | CA  | ILE | 59 | 89.207 | 79.005 | 76.118 | 1.00 | 21.26 |
| ATOM | 326 | CB  | ILE | 59 | 88.186 | 79.373 | 77.215 | 1.00 | 19.15 |
| ATOM | 327 | CG2 | ILE | 59 | 88.599 | 78.744 | 78.536 | 1.00 | 18.36 |
| ATOM | 328 | CG1 | ILE | 59 | 88.030 | 80.892 | 77.345 | 1.00 | 13.94 |
| ATOM | 329 | CD1 | ILE | 59 | 89.012 | 81.556 | 78.261 | 1.00 | 10.28 |
| ATOM | 330 | C   | ILE | 59 | 89.120 | 77.494 | 75.934 | 1.00 | 23.50 |
| ATOM | 331 | O   | ILE | 59 | 88.112 | 76.979 | 75.445 | 1.00 | 24.71 |
| ATOM | 332 | N   | THR | 60 | 90.163 | 76.784 | 76.335 | 1.00 | 22.69 |
| ATOM | 333 | CA  | THR | 60 | 90.182 | 75.337 | 76.211 | 1.00 | 22.98 |
| ATOM | 334 | CB  | THR | 60 | 91.067 | 74.904 | 75.028 | 1.00 | 26.30 |
| ATOM | 335 | OG1 | THR | 60 | 90.432 | 75.296 | 73.803 | 1.00 | 30.53 |
| ATOM | 336 | CG2 | THR | 60 | 91.283 | 73.398 | 75.026 | 1.00 | 27.27 |
| ATOM | 337 | C   | THR | 60 | 90.664 | 74.716 | 77.518 | 1.00 | 22.51 |
| ATOM | 338 | O   | THR | 60 | 91.712 | 75.080 | 78.038 | 1.00 | 25.19 |
| ATOM | 339 | N   | LEU | 61 | 89.865 | 73.806 | 78.057 | 1.00 | 20.62 |
| ATOM | 340 | CA  | LEU | 61 | 90.165 | 73.150 | 79.316 | 1.00 | 16.73 |
| ATOM | 341 | CB  | LEU | 61 | 88.910 | 73.162 | 80.190 | 1.00 | 14.48 |
| ATOM | 342 | CG  | LEU | 61 | 88.062 | 74.436 | 80.112 | 1.00 | 9.39  |
| ATOM | 343 | CD1 | LEU | 61 | 86.663 | 74.190 | 80.668 | 1.00 | 9.35  |
| ATOM | 344 | CD2 | LEU | 61 | 88.766 | 75.570 | 80.834 | 1.00 | 2.85  |
| ATOM | 345 | C   | LEU | 61 | 90.597 | 71.714 | 79.072 | 1.00 | 16.25 |

FIGURE 1 (CONT.)

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 346 | O   | LEU | 61 | 90.453 | 71.189 | 77.962 | 1.00 | 15.53 |
| ATOM | 347 | N   | LYS | 62 | 91.111 | 71.075 | 80.113 | 1.00 | 17.42 |
| ATOM | 348 | CA  | LYS | 62 | 91.550 | 69.695 | 80.017 | 1.00 | 20.31 |
| ATOM | 349 | CB  | LYS | 62 | 92.624 | 69.379 | 81.061 | 1.00 | 23.11 |
| ATOM | 350 | CG  | LYS | 62 | 93.910 | 70.206 | 80.915 | 1.00 | 31.56 |
| ATOM | 351 | CD  | LYS | 62 | 94.470 | 70.167 | 79.492 | 1.00 | 36.67 |
| ATOM | 352 | CE  | LYS | 62 | 94.867 | 68.753 | 79.074 | 1.00 | 40.37 |
| ATOM | 353 | NZ  | LYS | 62 | 95.167 | 68.655 | 77.613 | 1.00 | 41.00 |
| ATOM | 354 | C   | LYS | 62 | 90.360 | 68.773 | 80.190 | 1.00 | 22.22 |
| ATOM | 355 | O   | LYS | 62 | 90.378 | 67.642 | 79.718 | 1.00 | 24.32 |
| ATOM | 356 | N   | THR | 63 | 89.322 | 69.262 | 80.863 | 1.00 | 24.24 |
| ATOM | 357 | CA  | THR | 63 | 88.106 | 68.485 | 81.093 | 1.00 | 22.98 |
| ATOM | 358 | CB  | THR | 63 | 87.927 | 68.142 | 82.581 | 1.00 | 22.74 |
| ATOM | 359 | OG1 | THR | 63 | 87.737 | 69.344 | 83.327 | 1.00 | 28.60 |
| ATOM | 360 | CG2 | THR | 63 | 89.146 | 67.422 | 83.117 | 1.00 | 22.14 |
| ATOM | 361 | C   | THR | 63 | 86.913 | 69.312 | 80.621 | 1.00 | 22.76 |
| ATOM | 362 | O   | THR | 63 | 86.993 | 70.541 | 80.523 | 1.00 | 24.77 |
| ATOM | 363 | N   | PRO | 64 | 85.788 | 68.656 | 80.321 | 1.00 | 21.21 |
| ATOM | 364 | CD  | PRO | 64 | 85.600 | 67.195 | 80.223 | 1.00 | 20.66 |
| ATOM | 365 | CA  | PRO | 64 | 84.597 | 69.367 | 79.858 | 1.00 | 19.26 |
| ATOM | 366 | CB  | PRO | 64 | 83.938 | 68.321 | 78.974 | 1.00 | 20.57 |
| ATOM | 367 | CG  | PRO | 64 | 84.162 | 67.063 | 79.773 | 1.00 | 17.12 |
| ATOM | 368 | C   | PRO | 64 | 83.669 | 69.750 | 81.004 | 1.00 | 18.03 |
| ATOM | 369 | O   | PRO | 64 | 82.466 | 69.859 | 80.819 | 1.00 | 18.92 |
| ATOM | 370 | N   | LEU | 65 | 84.220 | 69.984 | 82.181 | 1.00 | 17.42 |
| ATOM | 371 | CA  | LEU | 65 | 83.388 | 70.281 | 83.331 | 1.00 | 17.61 |
| ATOM | 372 | CB  | LEU | 65 | 83.877 | 69.442 | 84.518 | 1.00 | 16.50 |
| ATOM | 373 | CG  | LEU | 65 | 84.124 | 67.954 | 84.216 | 1.00 | 11.41 |
| ATOM | 374 | CD1 | LEU | 65 | 84.753 | 67.288 | 85.403 | 1.00 | 10.97 |
| ATOM | 375 | CD2 | LEU | 65 | 82.840 | 67.245 | 83.834 | 1.00 | 9.50  |
| ATOM | 376 | C   | LEU | 65 | 83.326 | 71.769 | 83.679 | 1.00 | 18.70 |
| ATOM | 377 | O   | LEU | 65 | 84.331 | 72.472 | 83.605 | 1.00 | 19.19 |
| ATOM | 378 | N   | VAL | 66 | 82.145 | 72.234 | 84.081 | 1.00 | 16.36 |
| ATOM | 379 | CA  | VAL | 66 | 81.926 | 73.638 | 84.429 | 1.00 | 15.28 |
| ATOM | 380 | CB  | VAL | 66 | 81.328 | 74.418 | 83.206 | 1.00 | 14.14 |
| ATOM | 381 | CG1 | VAL | 66 | 81.133 | 75.878 | 83.547 | 1.00 | 13.24 |
| ATOM | 382 | CG2 | VAL | 66 | 82.221 | 74.291 | 81.985 | 1.00 | 12.95 |
| ATOM | 383 | C   | VAL | 66 | 80.927 | 73.740 | 85.595 | 1.00 | 14.30 |
| ATOM | 384 | O   | VAL | 66 | 79.938 | 73.018 | 85.624 | 1.00 | 15.07 |
| ATOM | 385 | N   | SER | 67 | 81.189 | 74.605 | 86.569 | 1.00 | 13.41 |
| ATOM | 386 | CA  | SER | 67 | 80.262 | 74.767 | 87.683 | 1.00 | 13.36 |
| ATOM | 387 | CB  | SER | 67 | 80.995 | 75.037 | 88.999 | 1.00 | 10.98 |
| ATOM | 388 | OG  | SER | 67 | 81.834 | 76.166 | 88.910 | 1.00 | 14.86 |
| ATOM | 389 | C   | SER | 67 | 79.322 | 75.909 | 87.330 | 1.00 | 14.70 |
| ATOM | 390 | O   | SER | 67 | 79.742 | 76.930 | 86.783 | 1.00 | 15.74 |
| ATOM | 391 | N   | SER | 68 | 78.041 | 75.718 | 87.610 | 1.00 | 15.87 |
| ATOM | 392 | CA  | SER | 68 | 77.022 | 76.706 | 87.293 | 1.00 | 16.05 |
| ATOM | 393 | CB  | SER | 68 | 75.639 | 76.067 | 87.443 | 1.00 | 18.67 |
| ATOM | 394 | OG  | SER | 68 | 74.602 | 77.004 | 87.194 | 1.00 | 21.96 |
| ATOM | 395 | C   | SER | 68 | 77.080 | 77.993 | 88.106 | 1.00 | 16.26 |
| ATOM | 396 | O   | SER | 68 | 77.445 | 77.995 | 89.283 | 1.00 | 16.76 |
| ATOM | 397 | N   | PRO | 69 | 76.699 | 79.116 | 87.483 | 1.00 | 16.03 |
| ATOM | 398 | CD  | PRO | 69 | 76.396 | 79.279 | 86.052 | 1.00 | 15.90 |
| ATOM | 399 | CA  | PRO | 69 | 76.699 | 80.411 | 88.169 | 1.00 | 15.65 |
| ATOM | 400 | CB  | PRO | 69 | 76.592 | 81.414 | 87.014 | 1.00 | 15.49 |
| ATOM | 401 | CG  | PRO | 69 | 76.975 | 80.626 | 85.778 | 1.00 | 17.02 |
| ATOM | 402 | C   | PRO | 69 | 75.445 | 80.475 | 89.063 | 1.00 | 16.27 |
| ATOM | 403 | O   | PRO | 69 | 74.384 | 80.927 | 88.625 | 1.00 | 13.16 |

FIGURE 1 (CONT.)

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 404 | N   | MET | 70 | 75.553 | 79.981 | 90.295 | 1.00 | 17.24 |
| ATOM | 405 | CA  | MET | 70 | 74.423 | 79.975 | 91.215 | 1.00 | 18.66 |
| ATOM | 406 | CB  | MET | 70 | 73.724 | 78.611 | 91.180 | 1.00 | 20.15 |
| ATOM | 407 | CG  | MET | 70 | 73.116 | 78.255 | 89.831 | 1.00 | 20.32 |
| ATOM | 408 | SD  | MET | 70 | 72.490 | 76.578 | 89.729 | 1.00 | 18.83 |
| ATOM | 409 | CE  | MET | 70 | 70.886 | 76.796 | 90.447 | 1.00 | 22.16 |
| ATOM | 410 | C   | MET | 70 | 74.868 | 80.270 | 92.633 | 1.00 | 19.79 |
| ATOM | 411 | O   | MET | 70 | 75.992 | 79.965 | 93.004 | 1.00 | 20.13 |
| ATOM | 412 | N   | ASP | 71 | 73.958 | 80.827 | 93.427 | 1.00 | 23.75 |
| ATOM | 413 | CA  | ASP | 71 | 74.194 | 81.184 | 94.832 | 1.00 | 24.77 |
| ATOM | 414 | CB  | ASP | 71 | 72.863 | 81.499 | 95.539 | 1.00 | 29.35 |
| ATOM | 415 | CG  | ASP | 71 | 72.367 | 82.882 | 95.265 | 1.00 | 38.41 |
| ATOM | 416 | OD1 | ASP | 71 | 73.156 | 83.834 | 95.406 | 1.00 | 47.71 |
| ATOM | 417 | OD2 | ASP | 71 | 71.177 | 83.021 | 94.930 | 1.00 | 44.52 |
| ATOM | 418 | C   | ASP | 71 | 74.842 | 80.080 | 95.643 | 1.00 | 22.82 |
| ATOM | 419 | O   | ASP | 71 | 75.774 | 80.331 | 96.404 | 1.00 | 23.85 |
| ATOM | 420 | N   | THR | 72 | 74.293 | 78.875 | 95.508 | 1.00 | 19.87 |
| ATOM | 421 | CA  | THR | 72 | 74.746 | 77.713 | 96.258 | 1.00 | 17.82 |
| ATOM | 422 | CB  | THR | 72 | 73.531 | 76.878 | 96.711 | 1.00 | 14.30 |
| ATOM | 423 | OG1 | THR | 72 | 72.808 | 76.423 | 95.562 | 1.00 | 13.27 |
| ATOM | 424 | CG2 | THR | 72 | 72.608 | 77.713 | 97.557 | 1.00 | 12.15 |
| ATOM | 425 | C   | THR | 72 | 75.725 | 76.792 | 95.534 | 1.00 | 17.18 |
| ATOM | 426 | O   | THR | 72 | 75.864 | 75.623 | 95.898 | 1.00 | 18.53 |
| ATOM | 427 | N   | VAL | 73 | 76.394 | 77.291 | 94.504 | 1.00 | 14.78 |
| ATOM | 428 | CA  | VAL | 73 | 77.317 | 76.440 | 93.786 | 1.00 | 13.05 |
| ATOM | 429 | CB  | VAL | 73 | 76.773 | 76.032 | 92.388 | 1.00 | 10.97 |
| ATOM | 430 | CG1 | VAL | 73 | 77.717 | 75.035 | 91.741 | 1.00 | 9.58  |
| ATOM | 431 | CG2 | VAL | 73 | 75.365 | 75.434 | 92.482 | 1.00 | 8.96  |
| ATOM | 432 | C   | VAL | 73 | 78.661 | 77.111 | 93.589 | 1.00 | 16.49 |
| ATOM | 433 | O   | VAL | 73 | 79.675 | 76.677 | 94.160 | 1.00 | 15.55 |
| ATOM | 434 | N   | THR | 74 | 78.650 | 78.223 | 92.860 | 1.00 | 17.15 |
| ATOM | 435 | CA  | THR | 74 | 79.894 | 78.896 | 92.539 | 1.00 | 18.39 |
| ATOM | 436 | CB  | THR | 74 | 80.096 | 78.965 | 91.011 | 1.00 | 17.98 |
| ATOM | 437 | OG1 | THR | 74 | 79.847 | 77.675 | 90.436 | 1.00 | 24.62 |
| ATOM | 438 | CG2 | THR | 74 | 81.531 | 79.368 | 90.675 | 1.00 | 19.70 |
| ATOM | 439 | C   | THR | 74 | 80.253 | 80.257 | 93.116 | 1.00 | 18.82 |
| ATOM | 440 | O   | THR | 74 | 79.606 | 81.274 | 92.847 | 1.00 | 20.11 |
| ATOM | 441 | N   | GLU | 75 | 81.354 | 80.247 | 93.854 | 1.00 | 18.87 |
| ATOM | 442 | CA  | GLU | 75 | 81.969 | 81.425 | 94.439 | 1.00 | 18.61 |
| ATOM | 443 | CB  | GLU | 75 | 81.534 | 81.645 | 95.886 | 1.00 | 14.35 |
| ATOM | 444 | CG  | GLU | 75 | 80.255 | 82.451 | 95.967 | 1.00 | 15.80 |
| ATOM | 445 | CD  | GLU | 75 | 79.843 | 82.834 | 97.379 | 1.00 | 21.75 |
| ATOM | 446 | OE1 | GLU | 75 | 80.413 | 82.310 | 98.363 | 1.00 | 26.31 |
| ATOM | 447 | OE2 | GLU | 75 | 78.917 | 83.664 | 97.505 | 1.00 | 20.92 |
| ATOM | 448 | C   | GLU | 75 | 83.469 | 81.131 | 94.301 | 1.00 | 19.83 |
| ATOM | 449 | O   | GLU | 75 | 83.847 | 80.171 | 93.619 | 1.00 | 19.89 |
| ATOM | 450 | N   | ALA | 76 | 84.326 | 81.934 | 94.919 | 1.00 | 20.57 |
| ATOM | 451 | CA  | ALA | 76 | 85.762 | 81.724 | 94.787 | 1.00 | 18.25 |
| ATOM | 452 | CB  | ALA | 76 | 86.517 | 82.637 | 95.713 | 1.00 | 22.39 |
| ATOM | 453 | C   | ALA | 76 | 86.178 | 80.278 | 95.008 | 1.00 | 17.57 |
| ATOM | 454 | O   | ALA | 76 | 86.733 | 79.652 | 94.110 | 1.00 | 18.52 |
| ATOM | 455 | N   | GLY | 77 | 85.845 | 79.739 | 96.177 | 1.00 | 16.64 |
| ATOM | 456 | CA  | GLY | 77 | 86.203 | 78.372 | 96.513 | 1.00 | 16.11 |
| ATOM | 457 | C   | GLY | 77 | 85.960 | 77.364 | 95.406 | 1.00 | 18.32 |
| ATOM | 458 | O   | GLY | 77 | 86.870 | 76.624 | 95.036 | 1.00 | 20.06 |
| ATOM | 459 | N   | MET | 78 | 84.744 | 77.345 | 94.866 | 1.00 | 19.25 |
| ATOM | 460 | CA  | MET | 78 | 84.381 | 76.420 | 93.797 | 1.00 | 17.27 |
| ATOM | 461 | CB  | MET | 78 | 82.878 | 76.495 | 93.501 | 1.00 | 14.83 |



FIGURE 1 (CONT.)

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 462 | CG  | MET | 78 | 82.379 | 75.543 | 92.416 | 1.00 | 9.04  |
| ATOM | 463 | SD  | MET | 78 | 82.630 | 73.797 | 92.794 | 1.00 | 9.74  |
| ATOM | 464 | CE  | MET | 78 | 81.306 | 73.505 | 93.947 | 1.00 | 4.67  |
| ATOM | 465 | C   | MET | 78 | 85.174 | 76.725 | 92.539 | 1.00 | 18.93 |
| ATOM | 466 | O   | MET | 78 | 85.817 | 75.835 | 91.985 | 1.00 | 20.73 |
| ATOM | 467 | N   | ALA | 79 | 85.173 | 77.990 | 92.122 | 1.00 | 19.92 |
| ATOM | 468 | CA  | ALA | 79 | 85.890 | 78.412 | 90.916 | 1.00 | 18.97 |
| ATOM | 469 | CB  | ALA | 79 | 85.761 | 79.919 | 90.715 | 1.00 | 17.50 |
| ATOM | 470 | C   | ALA | 79 | 87.357 | 78.002 | 90.955 | 1.00 | 19.41 |
| ATOM | 471 | O   | ALA | 79 | 87.912 | 77.573 | 89.949 | 1.00 | 21.40 |
| ATOM | 472 | N   | ILE | 80 | 87.977 | 78.106 | 92.125 | 1.00 | 20.17 |
| ATOM | 473 | CA  | ILE | 80 | 89.383 | 77.739 | 92.281 | 1.00 | 20.16 |
| ATOM | 474 | CB  | ILE | 80 | 89.964 | 78.235 | 93.641 | 1.00 | 18.57 |
| ATOM | 475 | CG2 | ILE | 80 | 91.349 | 77.658 | 93.385 | 1.00 | 16.92 |
| ATOM | 476 | CG1 | ILE | 80 | 90.034 | 79.758 | 93.662 | 1.00 | 19.76 |
| ATOM | 477 | CD1 | ILE | 80 | 90.403 | 80.338 | 95.011 | 1.00 | 22.90 |
| ATOM | 478 | C   | ILE | 80 | 89.547 | 76.228 | 92.188 | 1.00 | 19.90 |
| ATOM | 479 | O   | ILE | 80 | 90.330 | 75.740 | 91.381 | 1.00 | 19.26 |
| ATOM | 480 | N   | ALA | 81 | 88.773 | 75.496 | 92.984 | 1.00 | 20.78 |
| ATOM | 481 | CA  | ALA | 81 | 88.850 | 74.038 | 93.014 | 1.00 | 21.41 |
| ATOM | 482 | CB  | ALA | 81 | 87.876 | 73.479 | 94.027 | 1.00 | 22.18 |
| ATOM | 483 | C   | ALA | 81 | 88.586 | 73.439 | 91.653 | 1.00 | 22.24 |
| ATOM | 484 | O   | ALA | 81 | 89.308 | 72.544 | 91.210 | 1.00 | 25.18 |
| ATOM | 485 | N   | MET | 82 | 87.576 | 73.971 | 90.977 | 1.00 | 21.26 |
| ATOM | 486 | CA  | MET | 82 | 87.187 | 73.506 | 89.653 | 1.00 | 20.10 |
| ATOM | 487 | CB  | MET | 82 | 85.905 | 74.220 | 89.215 | 1.00 | 20.89 |
| ATOM | 488 | CG  | MET | 82 | 85.096 | 73.499 | 88.147 | 1.00 | 22.31 |
| ATOM | 489 | SD  | MET | 82 | 84.241 | 72.058 | 88.768 | 1.00 | 17.73 |
| ATOM | 490 | CE  | MET | 82 | 83.598 | 72.738 | 90.224 | 1.00 | 16.02 |
| ATOM | 491 | C   | MET | 82 | 88.307 | 73.740 | 88.628 | 1.00 | 18.83 |
| ATOM | 492 | O   | MET | 82 | 88.535 | 72.905 | 87.754 | 1.00 | 19.46 |
| ATOM | 493 | N   | ALA | 83 | 88.992 | 74.877 | 88.723 | 1.00 | 18.24 |
| ATOM | 494 | CA  | ALA | 83 | 90.082 | 75.184 | 87.801 | 1.00 | 17.87 |
| ATOM | 495 | CB  | ALA | 83 | 90.501 | 76.642 | 87.925 | 1.00 | 13.75 |
| ATOM | 496 | C   | ALA | 83 | 91.267 | 74.269 | 88.072 | 1.00 | 18.76 |
| ATOM | 497 | O   | ALA | 83 | 91.869 | 73.732 | 87.143 | 1.00 | 18.19 |
| ATOM | 498 | N   | LEU | 84 | 91.568 | 74.060 | 89.352 | 1.00 | 19.47 |
| ATOM | 499 | CA  | LEU | 84 | 92.687 | 73.213 | 89.754 | 1.00 | 19.62 |
| ATOM | 500 | CB  | LEU | 84 | 92.864 | 73.216 | 91.282 | 1.00 | 17.06 |
| ATOM | 501 | CG  | LEU | 84 | 93.341 | 74.485 | 92.011 | 1.00 | 14.41 |
| ATOM | 502 | CD1 | LEU | 84 | 93.302 | 74.256 | 93.508 | 1.00 | 9.31  |
| ATOM | 503 | CD2 | LEU | 84 | 94.742 | 74.893 | 91.579 | 1.00 | 10.69 |
| ATOM | 504 | C   | LEU | 84 | 92.518 | 71.778 | 89.268 | 1.00 | 22.34 |
| ATOM | 505 | O   | LEU | 84 | 93.503 | 71.089 | 88.986 | 1.00 | 24.52 |
| ATOM | 506 | N   | THR | 85 | 91.276 | 71.321 | 89.160 | 1.00 | 22.85 |
| ATOM | 507 | CA  | THR | 85 | 91.030 | 69.954 | 88.734 | 1.00 | 19.74 |
| ATOM | 508 | CB  | THR | 85 | 89.824 | 69.343 | 89.481 | 1.00 | 17.66 |
| ATOM | 509 | OG1 | THR | 85 | 88.669 | 70.165 | 89.301 | 1.00 | 16.20 |
| ATOM | 510 | CG2 | THR | 85 | 90.137 | 69.242 | 90.962 | 1.00 | 13.32 |
| ATOM | 511 | C   | THR | 85 | 90.927 | 69.748 | 87.232 | 1.00 | 19.88 |
| ATOM | 512 | O   | THR | 85 | 90.970 | 68.612 | 86.758 | 1.00 | 23.55 |
| ATOM | 513 | N   | GLY | 86 | 90.816 | 70.830 | 86.473 | 1.00 | 18.94 |
| ATOM | 514 | CA  | GLY | 86 | 90.744 | 70.689 | 85.030 | 1.00 | 16.63 |
| ATOM | 515 | C   | GLY | 86 | 89.580 | 71.388 | 84.362 | 1.00 | 18.45 |
| ATOM | 516 | O   | GLY | 86 | 89.538 | 71.457 | 83.129 | 1.00 | 21.10 |
| ATOM | 517 | N   | GLY | 87 | 88.615 | 71.852 | 85.151 | 1.00 | 16.36 |
| ATOM | 518 | CA  | GLY | 87 | 87.462 | 72.534 | 84.596 | 1.00 | 13.99 |
| ATOM | 519 | C   | GLY | 87 | 87.530 | 74.029 | 84.820 | 1.00 | 14.34 |

FIGURE 1 (CONT.)

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 520 | O   | GLY | 87 | 88.616 | 74.606 | 84.784 | 1.00 | 16.64 |
| ATOM | 521 | N   | ILE | 88 | 86.381 | 74.659 | 85.051 | 1.00 | 13.64 |
| ATOM | 522 | CA  | ILE | 88 | 86.315 | 76.097 | 85.292 | 1.00 | 14.14 |
| ATOM | 523 | CB  | ILE | 88 | 86.337 | 76.910 | 83.957 | 1.00 | 13.53 |
| ATOM | 524 | CG2 | ILE | 88 | 85.019 | 76.758 | 83.207 | 1.00 | 13.51 |
| ATOM | 525 | CG1 | ILE | 88 | 86.596 | 78.398 | 84.233 | 1.00 | 12.85 |
| ATOM | 526 | CD1 | ILE | 88 | 86.774 | 79.248 | 82.974 | 1.00 | 7.87  |
| ATOM | 527 | C   | ILE | 88 | 85.033 | 76.404 | 86.062 | 1.00 | 16.48 |
| ATOM | 528 | O   | ILE | 88 | 84.130 | 75.564 | 86.142 | 1.00 | 18.54 |
| ATOM | 529 | N   | GLY | 89 | 84.962 | 77.591 | 86.652 | 1.00 | 15.46 |
| ATOM | 530 | CA  | GLY | 89 | 83.775 | 77.965 | 87.389 | 1.00 | 14.33 |
| ATOM | 531 | C   | GLY | 89 | 83.293 | 79.336 | 86.965 | 1.00 | 15.78 |
| ATOM | 532 | O   | GLY | 89 | 84.073 | 80.128 | 86.430 | 1.00 | 16.51 |
| ATOM | 533 | N   | PHE | 90 | 81.997 | 79.584 | 87.145 | 1.00 | 15.87 |
| ATOM | 534 | CA  | PHE | 90 | 81.370 | 80.858 | 86.820 | 1.00 | 13.02 |
| ATOM | 535 | CB  | PHE | 90 | 80.302 | 80.671 | 85.748 | 1.00 | 10.44 |
| ATOM | 536 | CG  | PHE | 90 | 80.849 | 80.519 | 84.366 | 1.00 | 7.78  |
| ATOM | 537 | CD1 | PHE | 90 | 81.236 | 79.271 | 83.889 | 1.00 | 7.49  |
| ATOM | 538 | CD2 | PHE | 90 | 81.002 | 81.627 | 83.543 | 1.00 | 2.32  |
| ATOM | 539 | CE1 | PHE | 90 | 81.765 | 79.133 | 82.608 | 1.00 | 2.11  |
| ATOM | 540 | CE2 | PHE | 90 | 81.529 | 81.492 | 82.264 | 1.00 | 2.00  |
| ATOM | 541 | CZ  | PHE | 90 | 81.911 | 80.244 | 81.803 | 1.00 | 2.00  |
| ATOM | 542 | C   | PHE | 90 | 80.734 | 81.412 | 88.092 | 1.00 | 14.14 |
| ATOM | 543 | O   | PHE | 90 | 79.793 | 80.824 | 88.630 | 1.00 | 16.10 |
| ATOM | 544 | N   | ILE | 91 | 81.259 | 82.530 | 88.586 | 1.00 | 14.53 |
| ATOM | 545 | CA  | ILE | 91 | 80.740 | 83.147 | 89.810 | 1.00 | 12.62 |
| ATOM | 546 | CB  | ILE | 91 | 81.640 | 84.310 | 90.299 | 1.00 | 10.72 |
| ATOM | 547 | CG2 | ILE | 91 | 81.243 | 84.711 | 91.712 | 1.00 | 9.90  |
| ATOM | 548 | CG1 | ILE | 91 | 83.123 | 83.921 | 90.241 | 1.00 | 11.39 |
| ATOM | 549 | CD1 | ILE | 91 | 83.527 | 82.815 | 91.181 | 1.00 | 13.02 |
| ATOM | 550 | C   | ILE | 91 | 79.343 | 83.704 | 89.556 | 1.00 | 12.28 |
| ATOM | 551 | O   | ILE | 91 | 79.072 | 84.264 | 88.494 | 1.00 | 13.30 |
| ATOM | 552 | N   | HIS | 92 | 78.458 | 83.546 | 90.531 | 1.00 | 13.70 |
| ATOM | 553 | CA  | HIS | 92 | 77.093 | 84.044 | 90.407 | 1.00 | 13.81 |
| ATOM | 554 | CB  | HIS | 92 | 76.191 | 83.431 | 91.488 | 1.00 | 13.49 |
| ATOM | 555 | CG  | HIS | 92 | 76.413 | 83.993 | 92.859 | 1.00 | 11.95 |
| ATOM | 556 | CD2 | HIS | 92 | 75.949 | 85.118 | 93.448 | 1.00 | 10.24 |
| ATOM | 557 | ND1 | HIS | 92 | 77.183 | 83.358 | 93.808 | 1.00 | 16.02 |
| ATOM | 558 | CE1 | HIS | 92 | 77.183 | 84.063 | 94.924 | 1.00 | 12.53 |
| ATOM | 559 | NE2 | HIS | 92 | 76.442 | 85.137 | 94.731 | 1.00 | 14.71 |
| ATOM | 560 | C   | HIS | 92 | 77.088 | 85.567 | 90.527 | 1.00 | 13.18 |
| ATOM | 561 | O   | HIS | 92 | 78.006 | 86.150 | 91.087 | 1.00 | 13.75 |
| ATOM | 562 | N   | HIS | 93 | 76.043 | 86.205 | 90.020 | 1.00 | 13.84 |
| ATOM | 563 | CA  | HIS | 93 | 75.943 | 87.653 | 90.095 | 1.00 | 14.71 |
| ATOM | 564 | CB  | HIS | 93 | 75.788 | 88.276 | 88.705 | 1.00 | 17.81 |
| ATOM | 565 | CG  | HIS | 93 | 74.533 | 87.885 | 87.985 | 1.00 | 23.00 |
| ATOM | 566 | CD2 | HIS | 93 | 74.158 | 86.718 | 87.411 | 1.00 | 27.41 |
| ATOM | 567 | ND1 | HIS | 93 | 73.509 | 88.776 | 87.749 | 1.00 | 25.59 |
| ATOM | 568 | CE1 | HIS | 93 | 72.559 | 88.175 | 87.055 | 1.00 | 27.85 |
| ATOM | 569 | NE2 | HIS | 93 | 72.926 | 86.926 | 86.836 | 1.00 | 24.93 |
| ATOM | 570 | C   | HIS | 93 | 74.831 | 88.105 | 91.025 | 1.00 | 14.74 |
| ATOM | 571 | O   | HIS | 93 | 74.359 | 89.228 | 90.945 | 1.00 | 15.99 |
| ATOM | 572 | N   | ASN | 94 | 74.381 | 87.201 | 91.885 | 1.00 | 17.54 |
| ATOM | 573 | CA  | ASN | 94 | 73.340 | 87.516 | 92.860 | 1.00 | 18.66 |
| ATOM | 574 | CB  | ASN | 94 | 72.566 | 86.249 | 93.225 | 1.00 | 20.67 |
| ATOM | 575 | CG  | ASN | 94 | 71.413 | 86.516 | 94.175 | 1.00 | 22.98 |
| ATOM | 576 | OD1 | ASN | 94 | 71.278 | 85.849 | 95.199 | 1.00 | 27.48 |
| ATOM | 577 | ND2 | ASN | 94 | 70.552 | 87.456 | 93.810 | 1.00 | 19.79 |

FIGURE 1 (CONT.)

|      |     |     |     |     |        |        |        |      |       |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 578 | C   | ASN | 94  | 74.056 | 88.067 | 94.088 | 1.00 | 19.98 |
| ATOM | 579 | O   | ASN | 94  | 73.932 | 87.526 | 95.189 | 1.00 | 19.74 |
| ATOM | 580 | N   | CYS | 95  | 74.852 | 89.113 | 93.863 | 1.00 | 19.29 |
| ATOM | 581 | CA  | CYS | 95  | 75.637 | 89.783 | 94.896 | 1.00 | 20.12 |
| ATOM | 582 | CB  | CYS | 95  | 76.902 | 88.986 | 95.182 | 1.00 | 20.79 |
| ATOM | 583 | SG  | CYS | 95  | 77.831 | 88.599 | 93.694 | 1.00 | 23.06 |
| ATOM | 584 | C   | CYS | 95  | 76.014 | 91.152 | 94.343 | 1.00 | 22.11 |
| ATOM | 585 | O   | CYS | 95  | 75.616 | 91.490 | 93.228 | 1.00 | 24.36 |
| ATOM | 586 | N   | THR | 96  | 76.745 | 91.954 | 95.115 | 1.00 | 21.65 |
| ATOM | 587 | CA  | THR | 96  | 77.145 | 93.277 | 94.639 | 1.00 | 22.63 |
| ATOM | 588 | CB  | THR | 96  | 77.634 | 94.193 | 95.778 | 1.00 | 24.51 |
| ATOM | 589 | OG1 | THR | 96  | 78.672 | 93.540 | 96.520 | 1.00 | 29.99 |
| ATOM | 590 | CG2 | THR | 96  | 76.494 | 94.560 | 96.709 | 1.00 | 27.18 |
| ATOM | 591 | C   | THR | 96  | 78.271 | 93.155 | 93.628 | 1.00 | 22.82 |
| ATOM | 592 | O   | THR | 96  | 79.039 | 92.191 | 93.654 | 1.00 | 23.49 |
| ATOM | 593 | N   | PRO | 97  | 78.378 | 94.128 | 92.710 | 1.00 | 23.91 |
| ATOM | 594 | CD  | PRO | 97  | 77.427 | 95.220 | 92.438 | 1.00 | 23.87 |
| ATOM | 595 | CA  | PRO | 97  | 79.440 | 94.099 | 91.702 | 1.00 | 23.66 |
| ATOM | 596 | CB  | PRO | 97  | 79.250 | 95.433 | 90.989 | 1.00 | 22.66 |
| ATOM | 597 | CG  | PRO | 97  | 77.769 | 95.597 | 91.009 | 1.00 | 22.97 |
| ATOM | 598 | C   | PRO | 97  | 80.798 | 94.013 | 92.391 | 1.00 | 25.33 |
| ATOM | 599 | O   | PRO | 97  | 81.704 | 93.328 | 91.914 | 1.00 | 25.86 |
| ATOM | 600 | N   | GLU | 98  | 80.906 | 94.687 | 93.536 | 1.00 | 26.55 |
| ATOM | 601 | CA  | GLU | 98  | 82.126 | 94.703 | 94.344 | 1.00 | 28.76 |
| ATOM | 602 | CB  | GLU | 98  | 81.952 | 95.621 | 95.564 | 1.00 | 29.88 |
| ATOM | 603 | CG  | GLU | 98  | 81.732 | 97.096 | 95.255 | 1.00 | 38.55 |
| ATOM | 604 | CD  | GLU | 98  | 80.297 | 97.439 | 94.870 | 1.00 | 41.59 |
| ATOM | 605 | OE1 | GLU | 98  | 79.373 | 97.094 | 95.641 | 1.00 | 39.58 |
| ATOM | 606 | OE2 | GLU | 98  | 80.100 | 98.084 | 93.811 | 1.00 | 43.89 |
| ATOM | 607 | C   | GLU | 98  | 82.469 | 93.288 | 94.835 | 1.00 | 30.16 |
| ATOM | 608 | O   | GLU | 98  | 83.596 | 92.795 | 94.653 | 1.00 | 31.09 |
| ATOM | 609 | N   | PHE | 99  | 81.478 | 92.645 | 95.449 | 1.00 | 28.04 |
| ATOM | 610 | CA  | PHE | 99  | 81.619 | 91.302 | 95.989 | 1.00 | 24.81 |
| ATOM | 611 | CB  | PHE | 99  | 80.301 | 90.871 | 96.619 | 1.00 | 23.36 |
| ATOM | 612 | CG  | PHE | 99  | 80.334 | 89.502 | 97.235 | 1.00 | 24.63 |
| ATOM | 613 | CD1 | PHE | 99  | 80.695 | 89.335 | 98.563 | 1.00 | 26.18 |
| ATOM | 614 | CD2 | PHE | 99  | 79.951 | 88.384 | 96.502 | 1.00 | 21.79 |
| ATOM | 615 | CE1 | PHE | 99  | 80.668 | 88.075 | 99.159 | 1.00 | 26.07 |
| ATOM | 616 | CE2 | PHE | 99  | 79.922 | 87.132 | 97.088 | 1.00 | 20.62 |
| ATOM | 617 | CZ  | PHE | 99  | 80.282 | 86.975 | 98.422 | 1.00 | 22.53 |
| ATOM | 618 | C   | PHE | 99  | 82.004 | 90.322 | 94.905 | 1.00 | 23.00 |
| ATOM | 619 | O   | PHE | 99  | 82.969 | 89.577 | 95.052 | 1.00 | 23.86 |
| ATOM | 620 | N   | GLN | 100 | 81.249 | 90.336 | 93.813 | 1.00 | 21.74 |
| ATOM | 621 | CA  | GLN | 100 | 81.495 | 89.437 | 92.698 | 1.00 | 22.80 |
| ATOM | 622 | CB  | GLN | 100 | 80.488 | 89.671 | 91.581 | 1.00 | 22.40 |
| ATOM | 623 | CG  | GLN | 100 | 80.388 | 88.486 | 90.646 | 1.00 | 22.81 |
| ATOM | 624 | CD  | GLN | 100 | 79.585 | 88.781 | 89.417 | 1.00 | 21.83 |
| ATOM | 625 | OE1 | GLN | 100 | 79.391 | 89.941 | 89.051 | 1.00 | 25.98 |
| ATOM | 626 | NE2 | GLN | 100 | 79.120 | 87.739 | 88.758 | 1.00 | 19.59 |
| ATOM | 627 | C   | GLN | 100 | 82.900 | 89.608 | 92.154 | 1.00 | 23.30 |
| ATOM | 628 | O   | GLN | 100 | 83.625 | 88.626 | 91.951 | 1.00 | 23.42 |
| ATOM | 629 | N   | ALA | 101 | 83.281 | 90.859 | 91.920 | 1.00 | 24.22 |
| ATOM | 630 | CA  | ALA | 101 | 84.609 | 91.177 | 91.413 | 1.00 | 22.74 |
| ATOM | 631 | CB  | ALA | 101 | 84.725 | 92.669 | 91.159 | 1.00 | 21.49 |
| ATOM | 632 | C   | ALA | 101 | 85.689 | 90.706 | 92.395 | 1.00 | 22.04 |
| ATOM | 633 | O   | ALA | 101 | 86.759 | 90.265 | 91.982 | 1.00 | 20.44 |
| ATOM | 634 | N   | ASN | 102 | 85.399 | 90.769 | 93.691 | 1.00 | 22.30 |
| ATOM | 635 | CA  | ASN | 102 | 86.366 | 90.324 | 94.687 | 1.00 | 23.36 |

FIGURE 1 (CONT.)

|      |     |     |     |     |        |        |        |      |       |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 636 | CB  | ASN | 102 | 85.939 | 90.714 | 96.101 | 1.00 | 24.55 |
| ATOM | 637 | CG  | ASN | 102 | 86.996 | 90.378 | 97.142 | 1.00 | 27.11 |
| ATOM | 638 | OD1 | ASN | 102 | 88.152 | 90.789 | 97.028 | 1.00 | 29.62 |
| ATOM | 639 | ND2 | ASN | 102 | 86.602 | 89.629 | 98.165 | 1.00 | 27.00 |
| ATOM | 640 | C   | ASN | 102 | 86.511 | 88.817 | 94.594 | 1.00 | 25.46 |
| ATOM | 641 | O   | ASN | 102 | 87.604 | 88.277 | 94.797 | 1.00 | 28.34 |
| ATOM | 642 | N   | GLU | 103 | 85.408 | 88.134 | 94.294 | 1.00 | 25.42 |
| ATOM | 643 | CA  | GLU | 103 | 85.429 | 86.682 | 94.153 | 1.00 | 21.99 |
| ATOM | 644 | CB  | GLU | 103 | 84.009 | 86.126 | 94.011 | 1.00 | 22.69 |
| ATOM | 645 | CG  | GLU | 103 | 83.157 | 86.237 | 95.263 | 1.00 | 21.23 |
| ATOM | 646 | CD  | GLU | 103 | 83.850 | 85.685 | 96.492 | 1.00 | 22.96 |
| ATOM | 647 | OE1 | GLU | 103 | 83.874 | 84.451 | 96.667 | 1.00 | 17.62 |
| ATOM | 648 | OE2 | GLU | 103 | 84.382 | 86.493 | 97.281 | 1.00 | 29.03 |
| ATOM | 649 | C   | GLU | 103 | 86.278 | 86.304 | 92.940 | 1.00 | 20.97 |
| ATOM | 650 | O   | GLU | 103 | 86.985 | 85.299 | 92.966 | 1.00 | 22.40 |
| ATOM | 651 | N   | VAL | 104 | 86.217 | 87.116 | 91.887 | 1.00 | 18.20 |
| ATOM | 652 | CA  | VAL | 104 | 87.017 | 86.873 | 90.683 | 1.00 | 18.88 |
| ATOM | 653 | CB  | VAL | 104 | 86.620 | 87.824 | 89.521 | 1.00 | 17.86 |
| ATOM | 654 | CG1 | VAL | 104 | 87.427 | 87.506 | 88.255 | 1.00 | 16.68 |
| ATOM | 655 | CG2 | VAL | 104 | 85.138 | 87.722 | 89.245 | 1.00 | 17.68 |
| ATOM | 656 | C   | VAL | 104 | 88.493 | 87.104 | 91.019 | 1.00 | 19.92 |
| ATOM | 657 | O   | VAL | 104 | 89.355 | 86.302 | 90.666 | 1.00 | 21.70 |
| ATOM | 658 | N   | ARG | 105 | 88.764 | 88.189 | 91.737 | 1.00 | 21.51 |
| ATOM | 659 | CA  | ARG | 105 | 90.111 | 88.557 | 92.142 | 1.00 | 20.02 |
| ATOM | 660 | CB  | ARG | 105 | 90.067 | 89.879 | 92.889 | 1.00 | 22.18 |
| ATOM | 661 | CG  | ARG | 105 | 91.415 | 90.495 | 93.190 | 1.00 | 23.09 |
| ATOM | 662 | CD  | ARG | 105 | 91.260 | 91.639 | 94.184 | 1.00 | 25.23 |
| ATOM | 663 | NE  | ARG | 105 | 90.729 | 91.185 | 95.470 | 1.00 | 26.67 |
| ATOM | 664 | CZ  | ARG | 105 | 91.421 | 90.471 | 96.356 | 1.00 | 25.55 |
| ATOM | 665 | NH1 | ARG | 105 | 92.678 | 90.128 | 96.101 | 1.00 | 23.83 |
| ATOM | 666 | NH2 | ARG | 105 | 90.854 | 90.091 | 97.494 | 1.00 | 24.03 |
| ATOM | 667 | C   | ARG | 105 | 90.750 | 87.485 | 93.016 | 1.00 | 21.25 |
| ATOM | 668 | O   | ARG | 105 | 91.927 | 87.173 | 92.846 | 1.00 | 23.00 |
| ATOM | 669 | N   | LYS | 106 | 89.991 | 86.934 | 93.961 | 1.00 | 21.27 |
| ATOM | 670 | CA  | LYS | 106 | 90.511 | 85.879 | 94.837 | 1.00 | 23.38 |
| ATOM | 671 | CB  | LYS | 106 | 89.429 | 85.363 | 95.789 | 1.00 | 25.15 |
| ATOM | 672 | CG  | LYS | 106 | 89.012 | 86.317 | 96.883 | 1.00 | 26.05 |
| ATOM | 673 | CD  | LYS | 106 | 87.917 | 85.692 | 97.720 | 1.00 | 24.75 |
| ATOM | 674 | CE  | LYS | 106 | 87.424 | 86.662 | 98.761 | 1.00 | 29.64 |
| ATOM | 675 | NZ  | LYS | 106 | 86.273 | 86.122 | 99.528 | 1.00 | 31.16 |
| ATOM | 676 | C   | LYS | 106 | 90.988 | 84.705 | 93.992 | 1.00 | 25.07 |
| ATOM | 677 | O   | LYS | 106 | 92.099 | 84.199 | 94.174 | 1.00 | 25.83 |
| ATOM | 678 | N   | VAL | 107 | 90.119 | 84.269 | 93.084 | 1.00 | 25.62 |
| ATOM | 679 | CA  | VAL | 107 | 90.411 | 83.156 | 92.193 | 1.00 | 26.60 |
| ATOM | 680 | CB  | VAL | 107 | 89.172 | 82.815 | 91.313 | 1.00 | 29.16 |
| ATOM | 681 | CG1 | VAL | 107 | 89.529 | 81.801 | 90.242 | 1.00 | 34.41 |
| ATOM | 682 | CG2 | VAL | 107 | 88.066 | 82.255 | 92.175 | 1.00 | 28.28 |
| ATOM | 683 | C   | VAL | 107 | 91.622 | 83.488 | 91.323 | 1.00 | 26.84 |
| ATOM | 684 | O   | VAL | 107 | 92.581 | 82.713 | 91.272 | 1.00 | 27.67 |
| ATOM | 685 | N   | LYS | 108 | 91.602 | 84.662 | 90.694 | 1.00 | 25.49 |
| ATOM | 686 | CA  | LYS | 108 | 92.704 | 85.083 | 89.838 | 1.00 | 24.82 |
| ATOM | 687 | CB  | LYS | 108 | 92.386 | 86.418 | 89.155 | 1.00 | 22.18 |
| ATOM | 688 | CG  | LYS | 108 | 91.232 | 86.364 | 88.163 | 1.00 | 17.36 |
| ATOM | 689 | CD  | LYS | 108 | 91.391 | 85.228 | 87.161 | 1.00 | 13.78 |
| ATOM | 690 | CE  | LYS | 108 | 92.605 | 85.400 | 86.276 | 1.00 | 12.98 |
| ATOM | 691 | NZ  | LYS | 108 | 92.735 | 84.290 | 85.287 | 1.00 | 13.57 |
| ATOM | 692 | C   | LYS | 108 | 94.057 | 85.164 | 90.558 | 1.00 | 24.98 |
| ATOM | 693 | O   | LYS | 108 | 95.087 | 84.792 | 89.998 | 1.00 | 24.14 |

FIGURE 1 (CONT.)

|      |     |     |     |     |         |        |        |      |       |
|------|-----|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 694 | N   | LYS | 109 | 94.053  | 85.621 | 91.804 | 1.00 | 27.11 |
| ATOM | 695 | CA  | LYS | 109 | 95.284  | 85.746 | 92.579 | 1.00 | 28.48 |
| ATOM | 696 | CB  | LYS | 109 | 95.200  | 86.933 | 93.541 | 1.00 | 29.75 |
| ATOM | 697 | CG  | LYS | 109 | 95.849  | 88.195 | 93.020 | 1.00 | 31.35 |
| ATOM | 698 | CD  | LYS | 109 | 95.139  | 88.710 | 91.789 | 1.00 | 35.15 |
| ATOM | 699 | CE  | LYS | 109 | 95.870  | 89.897 | 91.196 | 1.00 | 40.43 |
| ATOM | 700 | NZ  | LYS | 109 | 97.184  | 89.511 | 90.621 | 1.00 | 41.81 |
| ATOM | 701 | C   | LYS | 109 | 95.651  | 84.503 | 93.369 | 1.00 | 29.07 |
| ATOM | 702 | O   | LYS | 109 | 96.618  | 84.520 | 94.123 | 1.00 | 33.10 |
| ATOM | 703 | N   | TYR | 110 | 94.891  | 83.430 | 93.219 | 1.00 | 29.29 |
| ATOM | 704 | CA  | TYR | 110 | 95.195  | 82.212 | 93.956 | 1.00 | 29.26 |
| ATOM | 705 | CB  | TYR | 110 | 94.086  | 81.186 | 93.770 | 1.00 | 23.08 |
| ATOM | 706 | CG  | TYR | 110 | 94.334  | 79.910 | 94.521 | 1.00 | 18.23 |
| ATOM | 707 | CD1 | TYR | 110 | 94.840  | 78.788 | 93.873 | 1.00 | 16.87 |
| ATOM | 708 | CE1 | TYR | 110 | 95.064  | 77.606 | 94.563 | 1.00 | 20.13 |
| ATOM | 709 | CD2 | TYR | 110 | 94.058  | 79.822 | 95.884 | 1.00 | 16.67 |
| ATOM | 710 | CE2 | TYR | 110 | 94.278  | 78.647 | 96.586 | 1.00 | 15.96 |
| ATOM | 711 | CZ  | TYR | 110 | 94.780  | 77.541 | 95.919 | 1.00 | 20.03 |
| ATOM | 712 | OH  | TYR | 110 | 94.994  | 76.366 | 96.605 | 1.00 | 24.77 |
| ATOM | 713 | C   | TYR | 110 | 96.541  | 81.605 | 93.551 | 1.00 | 31.47 |
| ATOM | 714 | O   | TYR | 110 | 97.252  | 81.042 | 94.381 | 1.00 | 30.19 |
| ATOM | 715 | N   | GLU | 111 | 96.865  | 81.693 | 92.268 | 1.00 | 33.91 |
| ATOM | 716 | CA  | GLU | 111 | 98.120  | 81.158 | 91.757 | 1.00 | 36.77 |
| ATOM | 717 | CB  | GLU | 111 | 97.881  | 79.801 | 91.087 | 1.00 | 39.21 |
| ATOM | 718 | CG  | GLU | 111 | 99.153  | 79.035 | 90.772 | 1.00 | 40.47 |
| ATOM | 719 | CD  | GLU | 111 | 98.894  | 77.697 | 90.115 | 1.00 | 40.03 |
| ATOM | 720 | OE1 | GLU | 111 | 97.978  | 76.970 | 90.552 | 1.00 | 36.17 |
| ATOM | 721 | OE2 | GLU | 111 | 99.623  | 77.367 | 89.160 | 1.00 | 47.17 |
| ATOM | 722 | C   | GLU | 111 | 98.627  | 82.177 | 90.746 | 1.00 | 37.77 |
| ATOM | 723 | O   | GLU | 111 | 97.867  | 82.622 | 89.886 | 1.00 | 36.85 |
| ATOM | 724 | N   | GLN | 112 | 99.901  | 82.546 | 90.847 | 1.00 | 39.85 |
| ATOM | 725 | CA  | GLN | 112 | 100.455 | 83.557 | 89.947 | 1.00 | 43.24 |
| ATOM | 726 | CB  | GLN | 112 | 100.630 | 84.872 | 90.709 | 1.00 | 44.65 |
| ATOM | 727 | CG  | GLN | 112 | 99.351  | 85.463 | 91.255 | 1.00 | 45.65 |
| ATOM | 728 | CD  | GLN | 112 | 99.615  | 86.631 | 92.169 | 1.00 | 48.62 |
| ATOM | 729 | OE1 | GLN | 112 | 100.161 | 87.656 | 91.749 | 1.00 | 51.83 |
| ATOM | 730 | NE2 | GLN | 112 | 99.243  | 86.484 | 93.433 | 1.00 | 48.44 |
| ATOM | 731 | C   | GLN | 112 | 101.768 | 83.239 | 89.236 | 1.00 | 43.51 |
| ATOM | 732 | O   | GLN | 112 | 101.930 | 83.530 | 88.048 | 1.00 | 43.39 |
| ATOM | 733 | N   | GLY | 113 | 102.727 | 82.694 | 89.972 | 1.00 | 43.98 |
| ATOM | 734 | CA  | GLY | 113 | 104.016 | 82.417 | 89.370 | 1.00 | 46.07 |
| ATOM | 735 | C   | GLY | 113 | 104.873 | 83.672 | 89.450 | 1.00 | 45.94 |
| ATOM | 736 | O   | GLY | 113 | 105.211 | 84.114 | 90.551 | 1.00 | 44.69 |
| ATOM | 737 | N   | PHE | 114 | 105.178 | 84.274 | 88.303 | 1.00 | 46.93 |
| ATOM | 738 | CA  | PHE | 114 | 106.012 | 85.476 | 88.258 | 1.00 | 49.84 |
| ATOM | 739 | CB  | PHE | 114 | 106.576 | 85.697 | 86.848 | 1.00 | 49.51 |
| ATOM | 740 | CG  | PHE | 114 | 107.780 | 84.853 | 86.538 | 1.00 | 53.18 |
| ATOM | 741 | CD1 | PHE | 114 | 109.002 | 85.113 | 87.147 | 1.00 | 54.85 |
| ATOM | 742 | CD2 | PHE | 114 | 107.690 | 83.786 | 85.653 | 1.00 | 55.88 |
| ATOM | 743 | CE1 | PHE | 114 | 110.116 | 84.320 | 86.883 | 1.00 | 54.76 |
| ATOM | 744 | CE2 | PHE | 114 | 108.801 | 82.986 | 85.383 | 1.00 | 57.03 |
| ATOM | 745 | CZ  | PHE | 114 | 110.017 | 83.256 | 86.002 | 1.00 | 56.60 |
| ATOM | 746 | C   | PHE | 114 | 105.284 | 86.729 | 88.714 | 1.00 | 52.11 |
| ATOM | 747 | O   | PHE | 114 | 104.750 | 87.471 | 87.889 | 1.00 | 54.09 |
| ATOM | 748 | N   | ILE | 115 | 105.289 | 86.986 | 90.018 | 1.00 | 53.71 |
| ATOM | 749 | CA  | ILE | 115 | 104.613 | 88.163 | 90.559 | 1.00 | 55.83 |
| ATOM | 750 | CB  | ILE | 115 | 104.342 | 88.018 | 92.092 | 1.00 | 56.93 |
| ATOM | 751 | CG2 | ILE | 115 | 103.879 | 86.587 | 92.409 | 1.00 | 54.73 |

FIGURE 1 (CONT.)

|      |     |    |     |     |         |         |         |      |        |
|------|-----|----|-----|-----|---------|---------|---------|------|--------|
| ATOM | 810 | CA | ALA | 131 | 115.979 | 91.696  | 103.320 | 1.00 | 83.91  |
| ATOM | 811 | N  | ALA | 132 | 116.601 | 91.294  | 101.015 | 1.00 | 81.04  |
| ATOM | 812 | CA | ALA | 132 | 117.423 | 91.354  | 99.810  | 1.00 | 80.28  |
| ATOM | 813 | CB | ALA | 132 | 116.642 | 90.807  | 98.627  | 1.00 | 80.36  |
| ATOM | 814 | C  | ALA | 132 | 117.962 | 92.740  | 99.476  | 1.00 | 80.39  |
| ATOM | 815 | O  | ALA | 132 | 117.357 | 93.757  | 99.820  | 1.00 | 80.20  |
| ATOM | 816 | N  | ALA | 133 | 119.116 | 92.771  | 98.819  | 1.00 | 80.93  |
| ATOM | 817 | CA | ALA | 133 | 119.746 | 94.022  | 98.414  | 1.00 | 81.53  |
| ATOM | 818 | CB | ALA | 133 | 121.079 | 94.193  | 99.123  | 1.00 | 80.70  |
| ATOM | 819 | C  | ALA | 133 | 119.942 | 94.038  | 96.902  | 1.00 | 82.58  |
| ATOM | 820 | O  | ALA | 133 | 121.026 | 94.358  | 96.414  | 1.00 | 82.75  |
| ATOM | 821 | N  | ALA | 134 | 118.887 | 93.681  | 96.173  | 1.00 | 83.81  |
| ATOM | 822 | CA | ALA | 134 | 118.921 | 93.629  | 94.711  | 1.00 | 83.39  |
| ATOM | 823 | CB | ALA | 134 | 117.965 | 92.545  | 94.198  | 1.00 | 82.19  |
| ATOM | 824 | C  | ALA | 134 | 118.568 | 94.980  | 94.097  | 1.00 | 82.93  |
| ATOM | 825 | O  | ALA | 134 | 119.388 | 95.912  | 94.241  | 1.00 | 82.67  |
| ATOM | 826 | CB | ALA | 150 | 120.001 | 97.614  | 89.743  | 1.00 | 101.69 |
| ATOM | 827 | C  | ALA | 150 | 118.719 | 98.142  | 91.821  | 1.00 | 100.94 |
| ATOM | 828 | O  | ALA | 150 | 117.883 | 97.395  | 92.335  | 1.00 | 100.35 |
| ATOM | 829 | N  | ALA | 150 | 120.213 | 96.186  | 91.749  | 1.00 | 101.14 |
| ATOM | 830 | CA | ALA | 150 | 120.017 | 97.577  | 91.261  | 1.00 | 101.10 |
| ATOM | 831 | N  | ALA | 151 | 118.540 | 99.452  | 91.659  | 1.00 | 101.13 |
| ATOM | 832 | CA | ALA | 151 | 117.370 | 100.181 | 92.157  | 1.00 | 100.24 |
| ATOM | 833 | CB | ALA | 151 | 116.061 | 99.469  | 91.761  | 1.00 | 100.01 |
| ATOM | 834 | C  | ALA | 151 | 117.505 | 100.323 | 93.681  | 1.00 | 98.83  |
| ATOM | 835 | O  | ALA | 151 | 118.409 | 101.018 | 94.154  | 1.00 | 99.01  |
| ATOM | 836 | N  | ALA | 152 | 116.644 | 99.649  | 94.440  | 1.00 | 96.46  |
| ATOM | 837 | CA | ALA | 152 | 116.703 | 99.696  | 95.902  | 1.00 | 92.96  |
| ATOM | 838 | CB | ALA | 152 | 116.218 | 101.052 | 96.416  | 1.00 | 93.49  |
| ATOM | 839 | C  | ALA | 152 | 115.857 | 98.567  | 96.484  | 1.00 | 90.09  |
| ATOM | 840 | O  | ALA | 152 | 115.387 | 98.644  | 97.620  | 1.00 | 89.57  |
| ATOM | 841 | N  | ALA | 153 | 115.715 | 97.496  | 95.710  | 1.00 | 87.27  |
| ATOM | 842 | CA | ALA | 153 | 114.922 | 96.345  | 96.118  | 1.00 | 85.11  |
| ATOM | 843 | CB | ALA | 153 | 115.035 | 95.242  | 95.089  | 1.00 | 87.03  |
| ATOM | 844 | C  | ALA | 153 | 115.297 | 95.820  | 97.497  | 1.00 | 83.27  |
| ATOM | 845 | O  | ALA | 153 | 116.343 | 95.190  | 97.687  | 1.00 | 82.09  |
| ATOM | 846 | N  | ALA | 154 | 114.438 | 96.116  | 98.464  | 1.00 | 82.07  |
| ATOM | 847 | CA | ALA | 154 | 114.633 | 95.680  | 99.838  | 1.00 | 79.91  |
| ATOM | 848 | CB | ALA | 154 | 113.774 | 96.528  | 100.784 | 1.00 | 80.13  |
| ATOM | 849 | C  | ALA | 154 | 114.308 | 94.188  | 100.000 | 1.00 | 77.83  |
| ATOM | 850 | O  | ALA | 154 | 114.751 | 93.551  | 100.963 | 1.00 | 77.74  |
| ATOM | 851 | N  | ALA | 155 | 113.533 | 93.640  | 99.066  | 1.00 | 74.67  |
| ATOM | 852 | CA | ALA | 155 | 113.145 | 92.231  | 99.083  | 1.00 | 71.48  |
| ATOM | 853 | CB | ALA | 155 | 112.173 | 91.958  | 100.221 | 1.00 | 70.07  |
| ATOM | 854 | C  | ALA | 155 | 112.518 | 91.835  | 97.752  | 1.00 | 70.62  |
| ATOM | 855 | O  | ALA | 155 | 112.036 | 92.752  | 97.053  | 1.00 | 68.84  |
| ATOM | 856 | CB | ALA | 178 | 117.058 | 95.505  | 102.209 | 1.00 | 58.93  |
| ATOM | 857 | C  | ALA | 178 | 119.494 | 95.204  | 102.731 | 1.00 | 57.03  |
| ATOM | 858 | O  | ALA | 178 | 120.605 | 95.013  | 102.255 | 1.00 | 55.07  |
| ATOM | 859 | N  | ALA | 178 | 118.804 | 95.985  | 100.513 | 1.00 | 59.48  |
| ATOM | 860 | CA | ALA | 178 | 118.475 | 96.029  | 101.962 | 1.00 | 58.59  |
| ATOM | 861 | N  | ALA | 179 | 119.102 | 94.724  | 103.907 | 1.00 | 57.92  |
| ATOM | 862 | CA | ALA | 179 | 119.967 | 93.936  | 104.773 | 1.00 | 60.34  |
| ATOM | 863 | CB | ALA | 179 | 119.171 | 93.363  | 105.938 | 1.00 | 61.38  |
| ATOM | 864 | C  | ALA | 179 | 120.710 | 92.832  | 104.044 | 1.00 | 61.59  |
| ATOM | 865 | O  | ALA | 179 | 121.839 | 93.038  | 103.606 | 1.00 | 61.85  |
| ATOM | 866 | N  | THR | 180 | 120.087 | 91.663  | 103.923 | 1.00 | 63.95  |
| ATOM | 867 | CA | THR | 180 | 120.718 | 90.536  | 103.245 | 1.00 | 65.71  |

FIGURE 1 (CONT.)

|      |     |     |     |     |         |         |         |      |        |
|------|-----|-----|-----|-----|---------|---------|---------|------|--------|
| ATOM | 752 | CG1 | ILE | 115 | 105.595 | 88.326  | 92.919  | 1.00 | 58.54  |
| ATOM | 753 | CD1 | ILE | 115 | 105.376 | 88.251  | 94.423  | 1.00 | 58.29  |
| ATOM | 754 | C   | ILE | 115 | 105.429 | 89.418  | 90.237  | 1.00 | 56.92  |
| ATOM | 755 | O   | ILE | 115 | 106.630 | 89.476  | 90.516  | 1.00 | 57.36  |
| ATOM | 756 | N   | THR | 116 | 104.788 | 90.399  | 89.605  | 1.00 | 58.66  |
| ATOM | 757 | CA  | THR | 116 | 105.474 | 91.633  | 89.222  | 1.00 | 61.25  |
| ATOM | 758 | CB  | THR | 116 | 105.077 | 92.065  | 87.797  | 1.00 | 60.84  |
| ATOM | 759 | OG1 | THR | 116 | 105.221 | 90.952  | 86.908  | 1.00 | 59.09  |
| ATOM | 760 | CG2 | THR | 116 | 105.966 | 93.213  | 87.312  | 1.00 | 62.79  |
| ATOM | 761 | C   | THR | 116 | 105.304 | 92.822  | 90.171  | 1.00 | 62.74  |
| ATOM | 762 | O   | THR | 116 | 106.278 | 93.470  | 90.538  | 1.00 | 62.00  |
| ATOM | 763 | N   | ASP | 117 | 104.067 | 93.118  | 90.553  | 1.00 | 65.44  |
| ATOM | 764 | CA  | ASP | 117 | 103.803 | 94.241  | 91.448  | 1.00 | 68.28  |
| ATOM | 765 | CB  | ASP | 117 | 102.351 | 94.209  | 91.959  | 1.00 | 70.75  |
| ATOM | 766 | CG  | ASP | 117 | 101.990 | 92.899  | 92.650  | 1.00 | 73.11  |
| ATOM | 767 | OD1 | ASP | 117 | 102.166 | 92.805  | 93.884  | 1.00 | 74.55  |
| ATOM | 768 | OD2 | ASP | 117 | 101.512 | 91.970  | 91.961  | 1.00 | 74.48  |
| ATOM | 769 | C   | ASP | 117 | 104.789 | 94.296  | 92.614  | 1.00 | 68.68  |
| ATOM | 770 | O   | ASP | 117 | 105.478 | 95.303  | 92.819  | 1.00 | 69.52  |
| ATOM | 771 | N   | ALA | 118 | 104.909 | 93.187  | 93.333  | 1.00 | 68.01  |
| ATOM | 772 | CA  | ALA | 118 | 105.812 | 93.131  | 94.466  | 1.00 | 67.77  |
| ATOM | 773 | CB  | ALA | 118 | 105.317 | 92.112  | 95.483  | 1.00 | 65.37  |
| ATOM | 774 | C   | ALA | 118 | 107.224 | 92.790  | 94.003  | 1.00 | 68.47  |
| ATOM | 775 | O   | ALA | 118 | 107.904 | 91.980  | 94.640  | 1.00 | 70.14  |
| ATOM | 776 | N   | ALA | 119 | 107.681 | 93.441  | 92.933  | 1.00 | 67.63  |
| ATOM | 777 | CA  | ALA | 119 | 109.021 | 93.204  | 92.399  | 1.00 | 65.42  |
| ATOM | 778 | CB  | ALA | 119 | 109.170 | 91.741  | 92.014  | 1.00 | 66.53  |
| ATOM | 779 | C   | ALA | 119 | 109.392 | 94.098  | 91.210  | 1.00 | 64.47  |
| ATOM | 780 | O   | ALA | 119 | 109.417 | 93.639  | 90.065  | 1.00 | 64.14  |
| ATOM | 781 | N   | ALA | 120 | 109.706 | 95.360  | 91.489  | 1.00 | 63.47  |
| ATOM | 782 | CA  | ALA | 120 | 110.098 | 96.316  | 90.452  | 1.00 | 62.64  |
| ATOM | 783 | CB  | ALA | 120 | 109.071 | 96.341  | 89.320  | 1.00 | 62.95  |
| ATOM | 784 | C   | ALA | 120 | 110.260 | 97.714  | 91.040  | 1.00 | 62.70  |
| ATOM | 785 | O   | ALA | 120 | 111.374 | 98.267  | 90.938  | 1.00 | 61.41  |
| ATOM | 786 | CB  | ALA | 125 | 109.000 | 94.859  | 98.198  | 1.00 | 153.76 |
| ATOM | 787 | C   | ALA | 125 | 109.160 | 95.344  | 95.747  | 1.00 | 153.51 |
| ATOM | 788 | O   | ALA | 125 | 109.902 | 94.992  | 94.829  | 1.00 | 153.54 |
| ATOM | 789 | N   | ALA | 125 | 109.423 | 93.056  | 96.557  | 1.00 | 154.27 |
| ATOM | 790 | CA  | ALA | 125 | 108.704 | 94.339  | 96.796  | 1.00 | 153.73 |
| ATOM | 791 | N   | ALA | 126 | 108.691 | 96.581  | 95.860  | 1.00 | 153.23 |
| ATOM | 792 | CA  | ALA | 126 | 109.075 | 97.621  | 94.916  | 1.00 | 153.16 |
| ATOM | 793 | CB  | ALA | 126 | 108.212 | 98.860  | 95.121  | 1.00 | 153.36 |
| ATOM | 794 | C   | ALA | 126 | 110.549 | 97.962  | 95.120  | 1.00 | 153.01 |
| ATOM | 795 | O   | ALA | 126 | 111.079 | 97.803  | 96.222  | 1.00 | 153.16 |
| ATOM | 796 | N   | ALA | 127 | 111.212 | 98.384  | 94.048  | 1.00 | 152.83 |
| ATOM | 797 | CA  | ALA | 127 | 112.621 | 98.754  | 94.114  | 1.00 | 152.63 |
| ATOM | 798 | CB  | ALA | 127 | 113.447 | 97.885  | 93.169  | 1.00 | 152.13 |
| ATOM | 799 | C   | ALA | 127 | 112.758 | 100.234 | 93.758  | 1.00 | 152.39 |
| ATOM | 800 | O   | ALA | 127 | 112.812 | 101.083 | 94.650  | 1.00 | 152.11 |
| ATOM | 801 | N   | ALA | 128 | 112.772 | 100.532 | 92.459  | 1.00 | 152.16 |
| ATOM | 802 | CA  | ALA | 128 | 112.884 | 101.901 | 91.953  | 1.00 | 151.90 |
| ATOM | 803 | CB  | ALA | 128 | 111.505 | 102.561 | 91.919  | 1.00 | 151.79 |
| ATOM | 804 | C   | ALA | 128 | 113.871 | 102.776 | 92.727  | 1.00 | 151.56 |
| ATOM | 805 | O   | ALA | 128 | 115.058 | 102.392 | 92.783  | 1.00 | 151.27 |
| ATOM | 806 | CB  | ALA | 131 | 115.610 | 90.226  | 103.503 | 1.00 | 85.15  |
| ATOM | 807 | C   | ALA | 131 | 116.950 | 91.870  | 102.162 | 1.00 | 82.41  |
| ATOM | 808 | O   | ALA | 131 | 117.960 | 92.557  | 102.293 | 1.00 | 82.59  |
| ATOM | 809 | N   | ALA | 131 | 114.753 | 92.513  | 103.126 | 1.00 | 84.45  |

FIGURE 1 (CONT.)

|      |     |     |     |     |         |        |         |      |       |
|------|-----|-----|-----|-----|---------|--------|---------|------|-------|
| ATOM | 868 | CB  | THR | 180 | 119.769 | 89.327 | 103.154 | 1.00 | 66.48 |
| ATOM | 869 | OG1 | THR | 180 | 119.034 | 89.205 | 104.381 | 1.00 | 66.35 |
| ATOM | 870 | CG2 | THR | 180 | 120.569 | 88.047 | 102.927 | 1.00 | 66.06 |
| ATOM | 871 | C   | THR | 180 | 121.139 | 90.989 | 101.851 | 1.00 | 66.16 |
| ATOM | 872 | O   | THR | 180 | 120.313 | 91.168 | 100.950 | 1.00 | 67.87 |
| ATOM | 873 | N   | LYS | 181 | 122.432 | 91.247 | 101.713 | 1.00 | 65.64 |
| ATOM | 874 | CA  | LYS | 181 | 122.995 | 91.718 | 100.463 | 1.00 | 64.54 |
| ATOM | 875 | CB  | LYS | 181 | 124.436 | 92.200 | 100.664 | 1.00 | 65.30 |
| ATOM | 876 | CG  | LYS | 181 | 125.255 | 91.387 | 101.658 | 1.00 | 66.54 |
| ATOM | 877 | CD  | LYS | 181 | 125.181 | 91.984 | 103.053 | 1.00 | 66.15 |
| ATOM | 878 | CE  | LYS | 181 | 125.741 | 93.398 | 103.078 | 1.00 | 65.67 |
| ATOM | 879 | NZ  | LYS | 181 | 125.692 | 93.970 | 104.451 | 1.00 | 68.13 |
| ATOM | 880 | C   | LYS | 181 | 122.921 | 90.750 | 99.291  | 1.00 | 63.31 |
| ATOM | 881 | O   | LYS | 181 | 122.910 | 89.522 | 99.456  | 1.00 | 63.71 |
| ATOM | 882 | N   | ARG | 182 | 122.872 | 91.339 | 98.101  | 1.00 | 61.46 |
| ATOM | 883 | CA  | ARG | 182 | 122.819 | 90.610 | 96.846  | 1.00 | 58.88 |
| ATOM | 884 | CB  | ARG | 182 | 122.421 | 91.564 | 95.716  | 1.00 | 54.15 |
| ATOM | 885 | CG  | ARG | 182 | 121.792 | 90.907 | 94.497  | 1.00 | 48.60 |
| ATOM | 886 | CD  | ARG | 182 | 122.610 | 89.741 | 94.004  | 1.00 | 43.01 |
| ATOM | 887 | NE  | ARG | 182 | 122.512 | 89.563 | 92.565  | 1.00 | 39.07 |
| ATOM | 888 | CZ  | ARG | 182 | 123.036 | 88.533 | 91.917  | 1.00 | 40.43 |
| ATOM | 889 | NH1 | ARG | 182 | 122.913 | 88.445 | 90.600  | 1.00 | 40.22 |
| ATOM | 890 | NH2 | ARG | 182 | 123.654 | 87.571 | 92.594  | 1.00 | 43.27 |
| ATOM | 891 | C   | ARG | 182 | 124.217 | 90.054 | 96.573  | 1.00 | 59.57 |
| ATOM | 892 | O   | ARG | 182 | 125.011 | 90.671 | 95.860  | 1.00 | 60.17 |
| ATOM | 893 | N   | GLU | 183 | 124.519 | 88.916 | 97.187  | 1.00 | 59.09 |
| ATOM | 894 | CA  | GLU | 183 | 125.801 | 88.231 | 97.025  | 1.00 | 59.57 |
| ATOM | 895 | CB  | GLU | 183 | 126.975 | 89.090 | 97.517  | 1.00 | 58.15 |
| ATOM | 896 | CG  | GLU | 183 | 126.849 | 89.602 | 98.937  | 1.00 | 57.54 |
| ATOM | 897 | CD  | GLU | 183 | 127.979 | 90.536 | 99.327  | 1.00 | 57.01 |
| ATOM | 898 | OE1 | GLU | 183 | 128.763 | 90.171 | 100.233 | 1.00 | 55.91 |
| ATOM | 899 | OE2 | GLU | 183 | 128.075 | 91.637 | 98.738  | 1.00 | 53.83 |
| ATOM | 900 | C   | GLU | 183 | 125.716 | 86.921 | 97.794  | 1.00 | 60.42 |
| ATOM | 901 | O   | GLU | 183 | 126.235 | 85.891 | 97.356  | 1.00 | 60.81 |
| ATOM | 902 | N   | ASP | 184 | 125.022 | 86.969 | 98.929  | 1.00 | 60.17 |
| ATOM | 903 | CA  | ASP | 184 | 124.815 | 85.793 | 99.765  | 1.00 | 59.99 |
| ATOM | 904 | CB  | ASP | 184 | 124.755 | 86.203 | 101.240 | 1.00 | 61.87 |
| ATOM | 905 | CG  | ASP | 184 | 126.073 | 86.771 | 101.743 | 1.00 | 64.92 |
| ATOM | 906 | OD1 | ASP | 184 | 126.328 | 87.976 | 101.538 | 1.00 | 67.44 |
| ATOM | 907 | OD2 | ASP | 184 | 126.856 | 85.008 | 102.349 | 1.00 | 65.08 |
| ATOM | 908 | C   | ASP | 184 | 123.499 | 85.119 | 99.348  | 1.00 | 59.20 |
| ATOM | 909 | O   | ASP | 184 | 123.287 | 83.925 | 99.590  | 1.00 | 59.14 |
| ATOM | 910 | N   | LEU | 185 | 122.649 | 85.897 | 98.677  | 1.00 | 57.41 |
| ATOM | 911 | CA  | LEU | 185 | 121.339 | 85.451 | 98.208  | 1.00 | 54.68 |
| ATOM | 912 | CB  | LEU | 185 | 120.368 | 86.630 | 98.202  | 1.00 | 59.34 |
| ATOM | 913 | CG  | LEU | 185 | 119.442 | 86.732 | 99.410  | 1.00 | 65.19 |
| ATOM | 914 | CD1 | LEU | 185 | 118.532 | 87.934 | 99.228  | 1.00 | 68.24 |
| ATOM | 915 | CD2 | LEU | 185 | 118.621 | 85.444 | 99.556  | 1.00 | 67.95 |
| ATOM | 916 | C   | LEU | 185 | 121.312 | 84.816 | 96.826  | 1.00 | 50.51 |
| ATOM | 917 | O   | LEU | 185 | 121.970 | 85.296 | 95.903  | 1.00 | 51.04 |
| ATOM | 918 | N   | VAL | 186 | 120.500 | 83.775 | 96.670  | 1.00 | 45.95 |
| ATOM | 919 | CA  | VAL | 186 | 120.373 | 83.120 | 95.373  | 1.00 | 41.48 |
| ATOM | 920 | CB  | VAL | 186 | 120.076 | 81.583 | 95.481  | 1.00 | 38.55 |
| ATOM | 921 | CG1 | VAL | 186 | 119.581 | 81.216 | 96.851  | 1.00 | 38.61 |
| ATOM | 922 | CG2 | VAL | 186 | 119.097 | 81.133 | 94.406  | 1.00 | 39.62 |
| ATOM | 923 | C   | VAL | 186 | 119.351 | 83.878 | 94.523  | 1.00 | 38.45 |
| ATOM | 924 | O   | VAL | 186 | 118.301 | 84.292 | 94.997  | 1.00 | 36.70 |
| ATOM | 925 | N   | VAL | 187 | 119.710 | 84.081 | 93.268  | 1.00 | 37.17 |



FIGURE 1 (CONT.)

|      |     |     |     |     |         |        |        |      |       |
|------|-----|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 926 | CA  | VAL | 187 | 118.910 | 84.821 | 92.316 | 1.00 | 35.95 |
| ATOM | 927 | CB  | VAL | 187 | 119.653 | 86.153 | 92.008 | 1.00 | 34.84 |
| ATOM | 928 | CG1 | VAL | 187 | 119.220 | 86.767 | 90.701 | 1.00 | 36.63 |
| ATOM | 929 | CG2 | VAL | 187 | 119.444 | 87.125 | 93.149 | 1.00 | 34.16 |
| ATOM | 930 | C   | VAL | 187 | 118.736 | 83.971 | 91.054 | 1.00 | 37.32 |
| ATOM | 931 | O   | VAL | 187 | 119.364 | 82.919 | 90.922 | 1.00 | 37.20 |
| ATOM | 932 | N   | ALA | 188 | 117.824 | 84.383 | 90.176 | 1.00 | 37.27 |
| ATOM | 933 | CA  | ALA | 188 | 117.579 | 83.687 | 88.924 | 1.00 | 38.14 |
| ATOM | 934 | CB  | ALA | 188 | 116.316 | 82.867 | 89.016 | 1.00 | 38.85 |
| ATOM | 935 | C   | ALA | 188 | 117.462 | 84.720 | 87.812 | 1.00 | 39.78 |
| ATOM | 936 | O   | ALA | 188 | 116.878 | 85.786 | 88.009 | 1.00 | 40.14 |
| ATOM | 937 | N   | PRO | 189 | 118.041 | 84.430 | 86.637 | 1.00 | 42.72 |
| ATOM | 938 | CD  | PRO | 189 | 118.817 | 83.213 | 86.349 | 1.00 | 42.66 |
| ATOM | 939 | CA  | PRO | 189 | 118.024 | 85.317 | 85.463 | 1.00 | 44.91 |
| ATOM | 940 | CB  | PRO | 189 | 118.901 | 84.563 | 84.454 | 1.00 | 42.51 |
| ATOM | 941 | CG  | PRO | 189 | 119.766 | 83.699 | 85.305 | 1.00 | 41.78 |
| ATOM | 942 | C   | PRO | 189 | 116.625 | 85.519 | 84.890 | 1.00 | 46.91 |
| ATOM | 943 | O   | PRO | 189 | 115.741 | 84.675 | 85.063 | 1.00 | 47.16 |
| ATOM | 944 | N   | ALA | 190 | 116.424 | 86.644 | 84.216 | 1.00 | 49.15 |
| ATOM | 945 | CA  | ALA | 190 | 115.139 | 86.925 | 83.589 | 1.00 | 52.79 |
| ATOM | 946 | CB  | ALA | 190 | 114.993 | 88.417 | 83.305 | 1.00 | 53.46 |
| ATOM | 947 | C   | ALA | 190 | 115.121 | 86.130 | 82.291 | 1.00 | 54.43 |
| ATOM | 948 | O   | ALA | 190 | 116.148 | 86.012 | 81.619 | 1.00 | 55.47 |
| ATOM | 949 | N   | GLY | 191 | 113.966 | 85.577 | 81.941 | 1.00 | 55.80 |
| ATOM | 950 | CA  | GLY | 191 | 113.873 | 84.792 | 80.727 | 1.00 | 57.80 |
| ATOM | 951 | C   | GLY | 191 | 113.784 | 83.309 | 81.033 | 1.00 | 59.83 |
| ATOM | 952 | O   | GLY | 191 | 113.512 | 82.502 | 80.142 | 1.00 | 61.79 |
| ATOM | 953 | N   | ILE | 192 | 114.052 | 82.932 | 82.280 | 1.00 | 60.59 |
| ATOM | 954 | CA  | ILE | 192 | 113.958 | 81.528 | 82.660 | 1.00 | 61.86 |
| ATOM | 955 | CB  | ILE | 192 | 114.564 | 81.224 | 84.062 | 1.00 | 61.08 |
| ATOM | 956 | CG2 | ILE | 192 | 116.035 | 81.594 | 84.101 | 1.00 | 62.19 |
| ATOM | 957 | CG1 | ILE | 192 | 113.773 | 81.933 | 85.164 | 1.00 | 59.47 |
| ATOM | 958 | CD1 | ILE | 192 | 114.135 | 81.476 | 86.552 | 1.00 | 57.49 |
| ATOM | 959 | C   | ILE | 192 | 112.481 | 81.175 | 82.692 | 1.00 | 63.40 |
| ATOM | 960 | O   | ILE | 192 | 111.626 | 82.016 | 82.416 | 1.00 | 63.75 |
| ATOM | 961 | N   | THR | 193 | 112.180 | 79.934 | 83.035 | 1.00 | 65.22 |
| ATOM | 962 | CA  | THR | 193 | 110.800 | 79.504 | 83.110 | 1.00 | 68.24 |
| ATOM | 963 | CB  | THR | 193 | 110.494 | 78.402 | 82.062 | 1.00 | 72.25 |
| ATOM | 964 | OG1 | THR | 193 | 109.082 | 78.122 | 82.046 | 1.00 | 75.84 |
| ATOM | 965 | CG2 | THR | 193 | 111.273 | 77.124 | 82.374 | 1.00 | 72.73 |
| ATOM | 966 | C   | THR | 193 | 110.536 | 78.993 | 84.519 | 1.00 | 68.78 |
| ATOM | 967 | O   | THR | 193 | 111.458 | 78.876 | 85.333 | 1.00 | 68.57 |
| ATOM | 968 | N   | LEU | 194 | 109.274 | 78.680 | 84.790 | 1.00 | 69.53 |
| ATOM | 969 | CA  | LEU | 194 | 108.848 | 78.179 | 86.089 | 1.00 | 70.58 |
| ATOM | 970 | CB  | LEU | 194 | 107.334 | 77.982 | 86.095 | 1.00 | 67.74 |
| ATOM | 971 | CG  | LEU | 194 | 106.529 | 79.277 | 86.033 | 1.00 | 62.43 |
| ATOM | 972 | CD1 | LEU | 194 | 105.081 | 78.958 | 85.786 | 1.00 | 62.21 |
| ATOM | 973 | CD2 | LEU | 194 | 106.697 | 80.049 | 87.328 | 1.00 | 60.58 |
| ATOM | 974 | C   | LEU | 194 | 109.557 | 76.885 | 86.480 | 1.00 | 72.55 |
| ATOM | 975 | O   | LEU | 194 | 109.900 | 76.687 | 87.651 | 1.00 | 72.45 |
| ATOM | 976 | N   | LYS | 195 | 109.770 | 76.006 | 85.502 | 1.00 | 74.70 |
| ATOM | 977 | CA  | LYS | 195 | 110.456 | 74.740 | 85.749 | 1.00 | 76.60 |
| ATOM | 978 | CB  | LYS | 195 | 110.556 | 73.916 | 84.459 | 1.00 | 77.31 |
| ATOM | 979 | CG  | LYS | 195 | 111.287 | 72.586 | 84.628 | 1.00 | 79.15 |
| ATOM | 980 | CD  | LYS | 195 | 110.574 | 71.695 | 85.640 | 1.00 | 81.61 |
| ATOM | 981 | CE  | LYS | 195 | 111.402 | 70.471 | 86.004 | 1.00 | 82.03 |
| ATOM | 982 | NZ  | LYS | 195 | 111.733 | 69.639 | 84.814 | 1.00 | 83.87 |
| ATOM | 983 | C   | LYS | 195 | 111.853 | 75.041 | 86.287 | 1.00 | 77.85 |

FIGURE 1 (CONT.)

|      |      |     |     |     |         |        |        |      |        |
|------|------|-----|-----|-----|---------|--------|--------|------|--------|
| ATOM | 984  | O   | LYS | 195 | 112.252 | 74.519 | 87.330 | 1.00 | 77.77  |
| ATOM | 985  | N   | GLU | 196 | 112.572 | 75.911 | 85.579 | 1.00 | 78.89  |
| ATOM | 986  | CA  | GLU | 196 | 113.920 | 76.312 | 85.968 | 1.00 | 79.64  |
| ATOM | 987  | CB  | GLU | 196 | 114.464 | 77.349 | 84.983 | 1.00 | 83.46  |
| ATOM | 988  | CG  | GLU | 196 | 114.576 | 76.850 | 83.547 | 1.00 | 90.70  |
| ATOM | 989  | CD  | GLU | 196 | 115.039 | 77.931 | 82.578 | 1.00 | 97.03  |
| ATOM | 990  | OE1 | GLU | 196 | 114.240 | 78.324 | 81.699 | 1.00 | 99.18  |
| ATOM | 991  | OE2 | GLU | 196 | 116.202 | 78.383 | 82.686 | 1.00 | 100.67 |
| ATOM | 992  | C   | GLU | 196 | 113.859 | 76.918 | 87.362 | 1.00 | 78.68  |
| ATOM | 993  | O   | GLU | 196 | 114.594 | 76.512 | 88.262 | 1.00 | 78.96  |
| ATOM | 994  | N   | ALA | 197 | 112.928 | 77.850 | 87.533 | 1.00 | 77.97  |
| ATOM | 995  | CA  | ALA | 197 | 112.707 | 78.556 | 88.789 | 1.00 | 77.86  |
| ATOM | 996  | CB  | ALA | 197 | 111.471 | 79.418 | 88.666 | 1.00 | 76.91  |
| ATOM | 997  | C   | ALA | 197 | 112.574 | 77.637 | 89.999 | 1.00 | 78.58  |
| ATOM | 998  | O   | ALA | 197 | 113.120 | 77.920 | 91.067 | 1.00 | 77.61  |
| ATOM | 999  | N   | ASN | 198 | 111.834 | 76.548 | 89.826 | 1.00 | 80.25  |
| ATOM | 1000 | CA  | ASN | 198 | 111.604 | 75.581 | 90.897 | 1.00 | 82.34  |
| ATOM | 1001 | CB  | ASN | 198 | 110.664 | 74.473 | 90.401 | 1.00 | 86.10  |
| ATOM | 1002 | CG  | ASN | 198 | 110.268 | 73.502 | 91.502 | 1.00 | 89.51  |
| ATOM | 1003 | OD1 | ASN | 198 | 110.999 | 72.559 | 91.811 | 1.00 | 91.70  |
| ATOM | 1004 | ND2 | ASN | 198 | 109.095 | 73.718 | 92.085 | 1.00 | 90.35  |
| ATOM | 1005 | C   | ASN | 198 | 112.898 | 74.968 | 91.429 | 1.00 | 81.89  |
| ATOM | 1006 | O   | ASN | 198 | 113.207 | 75.067 | 92.620 | 1.00 | 81.46  |
| ATOM | 1007 | N   | GLU | 199 | 113.666 | 74.360 | 90.533 | 1.00 | 81.93  |
| ATOM | 1008 | CA  | GLU | 199 | 114.914 | 73.719 | 90.907 | 1.00 | 82.51  |
| ATOM | 1009 | CB  | GLU | 199 | 115.504 | 72.990 | 89.701 | 1.00 | 84.93  |
| ATOM | 1010 | CG  | GLU | 199 | 116.740 | 72.168 | 90.020 | 1.00 | 91.19  |
| ATOM | 1011 | CD  | GLU | 199 | 117.236 | 71.365 | 88.829 | 1.00 | 95.27  |
| ATOM | 1012 | OE1 | GLU | 199 | 117.505 | 71.970 | 87.766 | 1.00 | 96.08  |
| ATOM | 1013 | OE2 | GLU | 199 | 117.356 | 70.126 | 88.962 | 1.00 | 97.16  |
| ATOM | 1014 | C   | GLU | 199 | 115.924 | 74.712 | 91.472 | 1.00 | 82.16  |
| ATOM | 1015 | O   | GLU | 199 | 116.461 | 74.496 | 92.562 | 1.00 | 82.41  |
| ATOM | 1016 | N   | ILE | 200 | 116.127 | 75.816 | 90.751 | 1.00 | 81.63  |
| ATOM | 1017 | CA  | ILE | 200 | 117.077 | 76.871 | 91.121 | 1.00 | 80.38  |
| ATOM | 1018 | CB  | ILE | 200 | 116.824 | 78.167 | 90.306 | 1.00 | 76.64  |
| ATOM | 1019 | CG2 | ILE | 200 | 117.588 | 79.349 | 90.897 | 1.00 | 75.73  |
| ATOM | 1020 | CG1 | ILE | 200 | 117.232 | 77.948 | 88.846 | 1.00 | 74.46  |
| ATOM | 1021 | CD1 | ILE | 200 | 116.991 | 79.141 | 87.945 | 1.00 | 74.00  |
| ATOM | 1022 | C   | ILE | 200 | 117.163 | 77.194 | 92.612 | 1.00 | 81.94  |
| ATOM | 1023 | O   | ILE | 200 | 118.217 | 77.596 | 93.100 | 1.00 | 83.53  |
| ATOM | 1024 | N   | LEU | 201 | 116.069 | 77.018 | 93.337 | 1.00 | 82.67  |
| ATOM | 1025 | CA  | LEU | 201 | 116.081 | 77.281 | 94.766 | 1.00 | 84.58  |
| ATOM | 1026 | CB  | LEU | 201 | 115.479 | 78.658 | 95.062 | 1.00 | 86.28  |
| ATOM | 1027 | CG  | LEU | 201 | 115.486 | 79.153 | 96.510 | 1.00 | 87.58  |
| ATOM | 1028 | CD1 | LEU | 201 | 116.907 | 79.183 | 97.046 | 1.00 | 85.65  |
| ATOM | 1029 | CD2 | LEU | 201 | 114.851 | 80.534 | 96.583 | 1.00 | 89.05  |
| ATOM | 1030 | C   | LEU | 201 | 115.289 | 76.180 | 95.443 | 1.00 | 85.36  |
| ATOM | 1031 | O   | LEU | 201 | 114.254 | 76.425 | 96.056 | 1.00 | 84.76  |
| ATOM | 1032 | N   | GLN | 202 | 115.785 | 74.956 | 95.332 | 1.00 | 87.32  |
| ATOM | 1033 | CA  | GLN | 202 | 115.097 | 73.823 | 95.927 | 1.00 | 89.77  |
| ATOM | 1034 | CB  | GLN | 202 | 115.698 | 72.501 | 95.445 | 1.00 | 92.70  |
| ATOM | 1035 | CG  | GLN | 202 | 114.824 | 71.290 | 95.764 | 1.00 | 97.61  |
| ATOM | 1036 | CD  | GLN | 202 | 113.358 | 71.499 | 95.387 | 1.00 | 101.05 |
| ATOM | 1037 | OE1 | GLN | 202 | 112.456 | 71.128 | 96.139 | 1.00 | 102.03 |
| ATOM | 1038 | NE2 | GLN | 202 | 113.120 | 72.105 | 94.229 | 1.00 | 102.67 |
| ATOM | 1039 | C   | GLN | 202 | 115.054 | 73.883 | 97.451 | 1.00 | 89.76  |
| ATOM | 1040 | O   | GLN | 202 | 115.836 | 73.222 | 98.142 | 1.00 | 90.00  |
| ATOM | 1041 | N   | ARG | 203 | 114.144 | 74.709 | 97.955 | 1.00 | 89.49  |

FIGURE 1 (CONT.)

|      |      |     |     |     |         |        |         |      |       |
|------|------|-----|-----|-----|---------|--------|---------|------|-------|
| ATOM | 1042 | CA  | ARG | 203 | 113.925 | 74.905 | 99.382  | 1.00 | 88.84 |
| ATOM | 1043 | CB  | ARG | 203 | 115.140 | 75.579 | 100.049 | 1.00 | 88.34 |
| ATOM | 1044 | CG  | ARG | 203 | 115.732 | 76.757 | 99.287  | 1.00 | 88.19 |
| ATOM | 1045 | CD  | ARG | 203 | 117.240 | 76.607 | 99.126  | 1.00 | 88.80 |
| ATOM | 1046 | NE  | ARG | 203 | 117.600 | 75.378 | 98.417  | 1.00 | 88.58 |
| ATOM | 1047 | CZ  | ARG | 203 | 118.428 | 75.317 | 97.377  | 1.00 | 86.71 |
| ATOM | 1048 | NH1 | ARG | 203 | 118.998 | 76.418 | 96.908  | 1.00 | 86.45 |
| ATOM | 1049 | NH2 | ARG | 203 | 118.687 | 74.146 | 96.809  | 1.00 | 85.61 |
| ATOM | 1050 | C   | ARG | 203 | 112.632 | 75.706 | 99.585  | 1.00 | 87.84 |
| ATOM | 1051 | O   | ARG | 203 | 111.566 | 75.287 | 99.121  | 1.00 | 87.56 |
| ATOM | 1052 | N   | ALA | 204 | 112.719 | 76.867 | 100.226 | 1.00 | 86.13 |
| ATOM | 1053 | CA  | ALA | 204 | 111.531 | 77.671 | 100.471 | 1.00 | 83.50 |
| ATOM | 1054 | CB  | ALA | 204 | 110.942 | 77.340 | 101.843 | 1.00 | 84.51 |
| ATOM | 1055 | C   | ALA | 204 | 111.815 | 79.165 | 100.358 | 1.00 | 80.44 |
| ATOM | 1056 | O   | ALA | 204 | 112.970 | 79.588 | 100.256 | 1.00 | 80.60 |
| ATOM | 1057 | N   | GLY | 205 | 110.744 | 79.952 | 100.384 | 1.00 | 76.39 |
| ATOM | 1058 | CA  | GLY | 205 | 110.859 | 81.392 | 100.283 | 1.00 | 69.88 |
| ATOM | 1059 | C   | GLY | 205 | 110.338 | 81.872 | 98.946  | 1.00 | 64.80 |
| ATOM | 1060 | O   | GLY | 205 | 109.236 | 81.511 | 98.515  | 1.00 | 64.06 |
| ATOM | 1061 | N   | ALA | 206 | 111.150 | 82.678 | 98.281  | 1.00 | 59.49 |
| ATOM | 1062 | CA  | ALA | 206 | 110.807 | 83.227 | 96.985  | 1.00 | 54.11 |
| ATOM | 1063 | CB  | ALA | 206 | 110.208 | 84.615 | 97.146  | 1.00 | 54.44 |
| ATOM | 1064 | C   | ALA | 206 | 112.108 | 83.310 | 96.226  | 1.00 | 49.90 |
| ATOM | 1065 | O   | ALA | 206 | 113.180 | 83.244 | 96.820  | 1.00 | 51.13 |
| ATOM | 1066 | N   | LEU | 209 | 112.026 | 83.413 | 94.912  | 1.00 | 45.11 |
| ATOM | 1067 | CA  | LEU | 209 | 113.225 | 83.517 | 94.111  | 1.00 | 40.05 |
| ATOM | 1068 | CB  | LEU | 209 | 113.239 | 82.427 | 93.048  | 1.00 | 36.41 |
| ATOM | 1069 | CG  | LEU | 209 | 114.558 | 81.773 | 92.645  | 1.00 | 34.85 |
| ATOM | 1070 | CD1 | LEU | 209 | 114.341 | 81.091 | 91.308  | 1.00 | 34.74 |
| ATOM | 1071 | CD2 | LEU | 209 | 115.691 | 82.771 | 92.546  | 1.00 | 29.56 |
| ATOM | 1072 | C   | LEU | 209 | 113.205 | 84.875 | 93.433  | 1.00 | 39.06 |
| ATOM | 1073 | O   | LEU | 209 | 112.312 | 85.153 | 92.634  | 1.00 | 39.13 |
| ATOM | 1074 | N   | PRO | 210 | 114.098 | 85.793 | 93.850  | 1.00 | 37.89 |
| ATOM | 1075 | CD  | PRO | 210 | 114.952 | 85.780 | 95.051  | 1.00 | 36.71 |
| ATOM | 1076 | CA  | PRO | 210 | 114.124 | 87.111 | 93.212  | 1.00 | 36.68 |
| ATOM | 1077 | CB  | PRO | 210 | 115.070 | 87.915 | 94.110  | 1.00 | 34.61 |
| ATOM | 1078 | CG  | PRO | 210 | 115.931 | 86.871 | 94.746  | 1.00 | 35.52 |
| ATOM | 1079 | C   | PRO | 210 | 114.656 | 86.987 | 91.786  | 1.00 | 36.86 |
| ATOM | 1080 | O   | PRO | 210 | 115.702 | 86.374 | 91.560  | 1.00 | 38.72 |
| ATOM | 1081 | N   | ILE | 211 | 113.889 | 87.477 | 90.818  | 1.00 | 35.16 |
| ATOM | 1082 | CA  | ILE | 211 | 114.316 | 87.415 | 89.432  | 1.00 | 33.61 |
| ATOM | 1083 | CB  | ILE | 211 | 113.131 | 87.224 | 88.473  | 1.00 | 31.67 |
| ATOM | 1084 | CG2 | ILE | 211 | 113.624 | 87.115 | 87.029  | 1.00 | 29.72 |
| ATOM | 1085 | CG1 | ILE | 211 | 112.373 | 85.953 | 88.852  | 1.00 | 26.60 |
| ATOM | 1086 | CD1 | ILE | 211 | 113.229 | 84.706 | 88.833  | 1.00 | 21.58 |
| ATOM | 1087 | C   | ILE | 211 | 115.036 | 88.709 | 89.147  | 1.00 | 34.69 |
| ATOM | 1088 | O   | ILE | 211 | 114.561 | 89.785 | 89.505  | 1.00 | 34.63 |
| ATOM | 1089 | N   | VAL | 212 | 116.189 | 88.597 | 88.506  | 1.00 | 37.32 |
| ATOM | 1090 | CA  | VAL | 212 | 117.016 | 89.750 | 88.209  | 1.00 | 41.26 |
| ATOM | 1091 | CB  | VAL | 212 | 118.393 | 89.593 | 88.910  | 1.00 | 39.76 |
| ATOM | 1092 | CG1 | VAL | 212 | 119.521 | 90.131 | 88.061  | 1.00 | 41.05 |
| ATOM | 1093 | CG2 | VAL | 212 | 118.357 | 90.286 | 90.264  | 1.00 | 36.94 |
| ATOM | 1094 | C   | VAL | 212 | 117.166 | 90.052 | 86.721  | 1.00 | 45.53 |
| ATOM | 1095 | O   | VAL | 212 | 117.324 | 89.149 | 85.898  | 1.00 | 46.04 |
| ATOM | 1096 | N   | ASN | 213 | 117.078 | 91.338 | 86.395  | 1.00 | 50.13 |
| ATOM | 1097 | CA  | ASN | 213 | 117.204 | 91.834 | 85.029  | 1.00 | 54.74 |
| ATOM | 1098 | CB  | ASN | 213 | 116.187 | 92.958 | 84.781  | 1.00 | 58.04 |
| ATOM | 1099 | CG  | ASN | 213 | 116.312 | 93.575 | 83.392  | 1.00 | 63.16 |

FIGURE 1 (CONT.)

|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 1100 | OD1 | ASN | 213 | 117.392 | 94.001 | 82.976 | 1.00 | 63.63 |
| ATOM | 1101 | ND2 | ASN | 213 | 115.195 | 93.644 | 82.676 | 1.00 | 66.53 |
| ATOM | 1102 | C   | ASN | 213 | 118.611 | 92.385 | 84.886 | 1.00 | 56.69 |
| ATOM | 1103 | O   | ASN | 213 | 119.049 | 93.171 | 85.728 | 1.00 | 56.84 |
| ATOM | 1104 | N   | GLU | 214 | 119.293 | 91.970 | 83.820 | 1.00 | 58.00 |
| ATOM | 1105 | CA  | GLU | 214 | 120.662 | 92.379 | 83.487 | 1.00 | 59.26 |
| ATOM | 1106 | CB  | GLU | 214 | 120.708 | 93.007 | 82.095 | 1.00 | 63.79 |
| ATOM | 1107 | CG  | GLU | 214 | 122.122 | 93.176 | 81.565 | 1.00 | 70.73 |
| ATOM | 1108 | CD  | GLU | 214 | 122.888 | 91.861 | 81.539 | 1.00 | 76.36 |
| ATOM | 1109 | OE1 | GLU | 214 | 123.897 | 91.739 | 82.273 | 1.00 | 77.43 |
| ATOM | 1110 | OE2 | GLU | 214 | 122.470 | 90.947 | 80.791 | 1.00 | 78.72 |
| ATOM | 1111 | C   | GLU | 214 | 121.381 | 93.296 | 84.471 | 1.00 | 58.22 |
| ATOM | 1112 | O   | GLU | 214 | 122.362 | 92.900 | 85.088 | 1.00 | 59.28 |
| ATOM | 1113 | N   | ASN | 215 | 120.873 | 94.507 | 84.647 | 1.00 | 57.43 |
| ATOM | 1114 | CA  | ASN | 215 | 121.482 | 95.458 | 85.567 | 1.00 | 58.14 |
| ATOM | 1115 | CB  | ASN | 215 | 120.804 | 96.828 | 85.450 | 1.00 | 65.27 |
| ATOM | 1116 | CG  | ASN | 215 | 120.970 | 97.459 | 84.073 | 1.00 | 74.29 |
| ATOM | 1117 | OD1 | ASN | 215 | 121.139 | 96.766 | 83.065 | 1.00 | 78.55 |
| ATOM | 1118 | ND2 | ASN | 215 | 120.909 | 98.786 | 84.024 | 1.00 | 77.85 |
| ATOM | 1119 | C   | ASN | 215 | 121.395 | 94.976 | 87.014 | 1.00 | 55.81 |
| ATOM | 1120 | O   | ASN | 215 | 121.650 | 95.747 | 87.945 | 1.00 | 56.29 |
| ATOM | 1121 | N   | ASP | 216 | 121.026 | 93.711 | 87.202 | 1.00 | 52.49 |
| ATOM | 1122 | CA  | ASP | 216 | 120.889 | 93.115 | 88.516 | 1.00 | 50.19 |
| ATOM | 1123 | CB  | ASP | 216 | 122.212 | 93.201 | 89.271 | 1.00 | 51.39 |
| ATOM | 1124 | CG  | ASP | 216 | 122.369 | 92.102 | 90.285 | 1.00 | 54.10 |
| ATOM | 1125 | OD1 | ASP | 216 | 121.951 | 92.299 | 91.445 | 1.00 | 57.69 |
| ATOM | 1126 | OD2 | ASP | 216 | 122.907 | 91.039 | 89.916 | 1.00 | 53.63 |
| ATOM | 1127 | C   | ASP | 216 | 119.769 | 93.852 | 89.247 | 1.00 | 49.43 |
| ATOM | 1128 | O   | ASP | 216 | 119.816 | 94.077 | 90.460 | 1.00 | 48.51 |
| ATOM | 1129 | N   | GLU | 217 | 118.757 | 94.234 | 88.478 | 1.00 | 50.39 |
| ATOM | 1130 | CA  | GLU | 217 | 117.600 | 94.959 | 88.994 | 1.00 | 51.67 |
| ATOM | 1131 | CB  | GLU | 217 | 117.268 | 96.126 | 88.054 | 1.00 | 56.48 |
| ATOM | 1132 | CG  | GLU | 217 | 117.200 | 95.734 | 86.571 | 1.00 | 62.18 |
| ATOM | 1133 | CD  | GLU | 217 | 117.162 | 96.933 | 85.631 | 1.00 | 67.67 |
| ATOM | 1134 | OE1 | GLU | 217 | 116.508 | 97.948 | 85.966 | 1.00 | 71.20 |
| ATOM | 1135 | OE2 | GLU | 217 | 117.785 | 96.858 | 84.550 | 1.00 | 67.88 |
| ATOM | 1136 | C   | GLU | 217 | 116.400 | 94.027 | 89.139 | 1.00 | 49.37 |
| ATOM | 1137 | O   | GLU | 217 | 116.063 | 93.296 | 88.203 | 1.00 | 50.54 |
| ATOM | 1138 | N   | LEU | 218 | 115.767 | 94.053 | 90.310 | 1.00 | 46.00 |
| ATOM | 1139 | CA  | LEU | 218 | 114.611 | 93.209 | 90.595 | 1.00 | 42.82 |
| ATOM | 1140 | CB  | LEU | 218 | 114.056 | 93.530 | 91.980 | 1.00 | 40.76 |
| ATOM | 1141 | CG  | LEU | 218 | 113.035 | 92.537 | 92.525 | 1.00 | 43.30 |
| ATOM | 1142 | CD1 | LEU | 218 | 113.587 | 91.125 | 92.443 | 1.00 | 45.66 |
| ATOM | 1143 | CD2 | LEU | 218 | 112.684 | 92.888 | 93.961 | 1.00 | 44.41 |
| ATOM | 1144 | C   | LEU | 218 | 113.530 | 93.392 | 89.539 | 1.00 | 41.76 |
| ATOM | 1145 | O   | LEU | 218 | 112.841 | 94.411 | 89.512 | 1.00 | 42.68 |
| ATOM | 1146 | N   | VAL | 219 | 113.395 | 92.399 | 88.665 | 1.00 | 40.13 |
| ATOM | 1147 | CA  | VAL | 219 | 112.414 | 92.447 | 87.582 | 1.00 | 35.68 |
| ATOM | 1148 | CB  | VAL | 219 | 113.056 | 91.969 | 86.234 | 1.00 | 32.66 |
| ATOM | 1149 | CG1 | VAL | 219 | 113.267 | 90.483 | 86.224 | 1.00 | 31.43 |
| ATOM | 1150 | CG2 | VAL | 219 | 112.223 | 92.386 | 85.057 | 1.00 | 34.92 |
| ATOM | 1151 | C   | VAL | 219 | 111.150 | 91.649 | 87.927 | 1.00 | 33.78 |
| ATOM | 1152 | O   | VAL | 219 | 110.092 | 91.864 | 87.337 | 1.00 | 34.95 |
| ATOM | 1153 | N   | ALA | 220 | 111.258 | 90.741 | 88.892 | 1.00 | 31.81 |
| ATOM | 1154 | CA  | ALA | 220 | 110.123 | 89.930 | 89.317 | 1.00 | 30.78 |
| ATOM | 1155 | CB  | ALA | 220 | 109.624 | 89.053 | 88.167 | 1.00 | 31.87 |
| ATOM | 1156 | C   | ALA | 220 | 110.538 | 89.062 | 90.486 | 1.00 | 29.91 |
| ATOM | 1157 | O   | ALA | 220 | 111.678 | 89.127 | 90.939 | 1.00 | 29.19 |

FIGURE 1 (CONT.)

|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 1158 | N   | ILE | 221 | 109.588 | 88.290 | 90.996 | 1.00 | 30.38 |
| ATOM | 1159 | CA  | ILE | 221 | 109.810 | 87.361 | 92.098 | 1.00 | 30.65 |
| ATOM | 1160 | CB  | ILE | 221 | 109.456 | 87.998 | 93.475 | 1.00 | 33.29 |
| ATOM | 1161 | CG2 | ILE | 221 | 109.558 | 86.974 | 94.587 | 1.00 | 35.92 |
| ATOM | 1162 | CG1 | ILE | 221 | 110.430 | 89.126 | 93.814 | 1.00 | 36.90 |
| ATOM | 1163 | CD1 | ILE | 221 | 110.282 | 89.662 | 95.232 | 1.00 | 39.70 |
| ATOM | 1164 | C   | ILE | 221 | 108.891 | 86.166 | 91.830 | 1.00 | 30.07 |
| ATOM | 1165 | O   | ILE | 221 | 108.010 | 86.242 | 90.976 | 1.00 | 29.66 |
| ATOM | 1166 | N   | ILE | 222 | 109.158 | 85.043 | 92.486 | 1.00 | 30.43 |
| ATOM | 1167 | CA  | ILE | 222 | 108.339 | 83.843 | 92.352 | 1.00 | 32.62 |
| ATOM | 1168 | CB  | ILE | 222 | 108.885 | 82.873 | 91.281 | 1.00 | 35.84 |
| ATOM | 1169 | CG2 | ILE | 222 | 108.282 | 83.173 | 89.929 | 1.00 | 38.08 |
| ATOM | 1170 | CG1 | ILE | 222 | 110.403 | 82.948 | 91.225 | 1.00 | 40.71 |
| ATOM | 1171 | CD1 | ILE | 222 | 110.979 | 82.332 | 89.992 | 1.00 | 48.17 |
| ATOM | 1172 | C   | ILE | 222 | 108.307 | 83.143 | 93.699 | 1.00 | 32.70 |
| ATOM | 1173 | O   | ILE | 222 | 109.336 | 82.696 | 94.202 | 1.00 | 32.91 |
| ATOM | 1174 | N   | ALA | 223 | 107.131 | 83.096 | 94.304 | 1.00 | 34.15 |
| ATOM | 1175 | CA  | ALA | 223 | 106.971 | 82.469 | 95.606 | 1.00 | 36.37 |
| ATOM | 1176 | CB  | ALA | 223 | 105.677 | 82.936 | 96.253 | 1.00 | 40.47 |
| ATOM | 1177 | C   | ALA | 223 | 106.981 | 80.962 | 95.481 | 1.00 | 36.88 |
| ATOM | 1178 | O   | ALA | 223 | 106.339 | 80.408 | 94.592 | 1.00 | 38.29 |
| ATOM | 1179 | N   | ARG | 224 | 107.683 | 80.300 | 96.393 | 1.00 | 37.92 |
| ATOM | 1180 | CA  | ARG | 224 | 107.778 | 78.842 | 96.378 | 1.00 | 39.64 |
| ATOM | 1181 | CB  | ARG | 224 | 108.533 | 78.336 | 97.623 | 1.00 | 40.36 |
| ATOM | 1182 | CG  | ARG | 224 | 109.850 | 77.565 | 97.349 | 1.00 | 43.06 |
| ATOM | 1183 | CD  | ARG | 224 | 111.088 | 78.471 | 97.101 | 1.00 | 43.23 |
| ATOM | 1184 | NE  | ARG | 224 | 111.056 | 79.161 | 95.809 | 1.00 | 41.83 |
| ATOM | 1185 | CZ  | ARG | 224 | 111.816 | 78.842 | 94.765 | 1.00 | 37.49 |
| ATOM | 1186 | NH1 | ARG | 224 | 112.680 | 77.847 | 94.848 | 1.00 | 33.15 |
| ATOM | 1187 | NH2 | ARG | 224 | 111.678 | 79.492 | 93.619 | 1.00 | 38.85 |
| ATOM | 1188 | C   | ARG | 224 | 106.386 | 78.210 | 96.316 | 1.00 | 40.65 |
| ATOM | 1189 | O   | ARG | 224 | 106.154 | 77.288 | 95.535 | 1.00 | 41.59 |
| ATOM | 1190 | N   | THR | 225 | 105.446 | 78.768 | 97.076 | 1.00 | 42.15 |
| ATOM | 1191 | CA  | THR | 225 | 104.072 | 78.264 | 97.136 | 1.00 | 42.10 |
| ATOM | 1192 | CB  | THR | 225 | 103.201 | 79.140 | 98.056 | 1.00 | 41.51 |
| ATOM | 1193 | OG1 | THR | 225 | 103.319 | 80.515 | 97.667 | 1.00 | 42.81 |
| ATOM | 1194 | CG2 | THR | 225 | 103.651 | 78.995 | 99.501 | 1.00 | 40.52 |
| ATOM | 1195 | C   | THR | 225 | 103.391 | 78.119 | 95.772 | 1.00 | 43.03 |
| ATOM | 1196 | O   | THR | 225 | 102.639 | 77.170 | 95.545 | 1.00 | 43.47 |
| ATOM | 1197 | N   | ASP | 226 | 103.658 | 79.051 | 94.866 | 1.00 | 43.78 |
| ATOM | 1198 | CA  | ASP | 226 | 103.075 | 78.991 | 93.535 | 1.00 | 44.84 |
| ATOM | 1199 | CB  | ASP | 226 | 103.324 | 80.296 | 92.775 | 1.00 | 48.02 |
| ATOM | 1200 | CG  | ASP | 226 | 102.595 | 81.473 | 93.383 | 1.00 | 52.98 |
| ATOM | 1201 | OD1 | ASP | 226 | 101.569 | 81.264 | 94.073 | 1.00 | 55.78 |
| ATOM | 1202 | OD2 | ASP | 226 | 103.051 | 82.616 | 93.166 | 1.00 | 58.70 |
| ATOM | 1203 | C   | ASP | 226 | 103.647 | 77.811 | 92.760 | 1.00 | 44.39 |
| ATOM | 1204 | O   | ASP | 226 | 102.919 | 77.102 | 92.064 | 1.00 | 46.30 |
| ATOM | 1205 | N   | LEU | 227 | 104.951 | 77.594 | 92.895 | 1.00 | 42.85 |
| ATOM | 1206 | CA  | LEU | 227 | 105.617 | 76.488 | 92.211 | 1.00 | 41.91 |
| ATOM | 1207 | CB  | LEU | 227 | 107.127 | 76.573 | 92.418 | 1.00 | 41.83 |
| ATOM | 1208 | CG  | LEU | 227 | 107.875 | 77.618 | 91.581 | 1.00 | 43.67 |
| ATOM | 1209 | CD1 | LEU | 227 | 107.080 | 78.906 | 91.413 | 1.00 | 44.20 |
| ATOM | 1210 | CD2 | LEU | 227 | 109.207 | 77.911 | 92.234 | 1.00 | 45.65 |
| ATOM | 1211 | C   | LEU | 227 | 105.060 | 75.161 | 92.727 | 1.00 | 41.23 |
| ATOM | 1212 | O   | LEU | 227 | 105.052 | 74.159 | 92.008 | 1.00 | 40.43 |
| ATOM | 1213 | N   | LYS | 228 | 104.581 | 75.173 | 93.969 | 1.00 | 41.25 |
| ATOM | 1214 | CA  | LYS | 228 | 103.976 | 74.002 | 94.598 | 1.00 | 41.51 |
| ATOM | 1215 | CB  | LYS | 228 | 103.801 | 74.242 | 96.103 | 1.00 | 42.68 |

FIGURE 1 (CONT.)

|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 1216 | CG  | LYS | 228 | 103.048 | 73.147 | 96.844 | 1.00 | 47.59 |
| ATOM | 1217 | CD  | LYS | 228 | 102.737 | 73.585 | 98.272 | 1.00 | 53.52 |
| ATOM | 1218 | CE  | LYS | 228 | 101.781 | 72.623 | 98.978 | 1.00 | 56.97 |
| ATOM | 1219 | NZ  | LYS | 228 | 102.353 | 71.257 | 99.167 | 1.00 | 59.90 |
| ATOM | 1220 | C   | LYS | 228 | 102.615 | 73.737 | 93.948 | 1.00 | 40.91 |
| ATOM | 1221 | O   | LYS | 228 | 102.390 | 72.664 | 93.386 | 1.00 | 41.81 |
| ATOM | 1222 | N   | LYS | 229 | 101.735 | 74.738 | 93.985 | 1.00 | 38.16 |
| ATOM | 1223 | CA  | LYS | 229 | 100.392 | 74.627 | 93.412 | 1.00 | 36.08 |
| ATOM | 1224 | CB  | LYS | 229 | 99.648  | 75.958 | 93.524 | 1.00 | 34.26 |
| ATOM | 1225 | CG  | LYS | 229 | 99.472  | 76.460 | 94.936 | 1.00 | 32.34 |
| ATOM | 1226 | CD  | LYS | 229 | 98.862  | 77.842 | 94.945 | 1.00 | 33.74 |
| ATOM | 1227 | CE  | LYS | 229 | 98.789  | 78.398 | 96.358 | 1.00 | 36.97 |
| ATOM | 1228 | NZ  | LYS | 229 | 98.186  | 79.757 | 96.400 | 1.00 | 37.99 |
| ATOM | 1229 | C   | LYS | 229 | 100.475 | 74.236 | 91.946 | 1.00 | 36.73 |
| ATOM | 1230 | O   | LYS | 229 | 99.659  | 73.457 | 91.446 | 1.00 | 36.54 |
| ATOM | 1231 | N   | ASN | 230 | 101.459 | 74.790 | 91.254 | 1.00 | 36.88 |
| ATOM | 1232 | CA  | ASN | 230 | 101.637 | 74.483 | 89.852 | 1.00 | 38.77 |
| ATOM | 1233 | CB  | ASN | 230 | 102.698 | 75.386 | 89.229 | 1.00 | 40.52 |
| ATOM | 1234 | CG  | ASN | 230 | 102.822 | 75.191 | 87.721 | 1.00 | 47.50 |
| ATOM | 1235 | OD1 | ASN | 230 | 103.865 | 75.473 | 87.135 | 1.00 | 49.21 |
| ATOM | 1236 | ND2 | ASN | 230 | 101.754 | 74.710 | 87.086 | 1.00 | 52.48 |
| ATOM | 1237 | C   | ASN | 230 | 102.019 | 73.025 | 89.652 | 1.00 | 40.23 |
| ATOM | 1238 | O   | ASN | 230 | 101.474 | 72.360 | 88.773 | 1.00 | 42.09 |
| ATOM | 1239 | N   | ARG | 231 | 102.923 | 72.522 | 90.488 | 1.00 | 40.83 |
| ATOM | 1240 | CA  | ARG | 231 | 103.389 | 71.141 | 90.377 | 1.00 | 41.51 |
| ATOM | 1241 | CB  | ARG | 231 | 104.734 | 70.975 | 91.106 | 1.00 | 47.17 |
| ATOM | 1242 | CG  | ARG | 231 | 105.495 | 69.686 | 90.773 | 1.00 | 54.46 |
| ATOM | 1243 | CD  | ARG | 231 | 106.892 | 69.674 | 91.405 | 1.00 | 66.37 |
| ATOM | 1244 | NE  | ARG | 231 | 107.667 | 68.482 | 91.043 | 1.00 | 76.11 |
| ATOM | 1245 | CZ  | ARG | 231 | 108.942 | 68.267 | 91.378 | 1.00 | 78.92 |
| ATOM | 1246 | NH1 | ARG | 231 | 109.544 | 67.149 | 90.992 | 1.00 | 79.85 |
| ATOM | 1247 | NH2 | ARG | 231 | 109.621 | 69.156 | 92.100 | 1.00 | 78.17 |
| ATOM | 1248 | C   | ARG | 231 | 102.366 | 70.126 | 90.892 | 1.00 | 38.99 |
| ATOM | 1249 | O   | ARG | 231 | 102.328 | 68.976 | 90.442 | 1.00 | 37.79 |
| ATOM | 1250 | N   | ASP | 232 | 101.525 | 70.565 | 91.820 | 1.00 | 36.95 |
| ATOM | 1251 | CA  | ASP | 232 | 100.509 | 69.700 | 92.405 | 1.00 | 35.45 |
| ATOM | 1252 | CB  | ASP | 232 | 100.007 | 70.287 | 93.730 | 1.00 | 40.00 |
| ATOM | 1253 | CG  | ASP | 232 | 101.014 | 70.149 | 94.860 | 1.00 | 46.07 |
| ATOM | 1254 | OD1 | ASP | 232 | 102.209 | 69.902 | 94.588 | 1.00 | 48.49 |
| ATOM | 1255 | OD2 | ASP | 232 | 100.600 | 70.293 | 96.033 | 1.00 | 50.50 |
| ATOM | 1256 | C   | ASP | 232 | 99.312  | 69.463 | 91.486 | 1.00 | 32.77 |
| ATOM | 1257 | O   | ASP | 232 | 98.687  | 68.405 | 91.541 | 1.00 | 32.41 |
| ATOM | 1258 | N   | TYR | 233 | 98.986  | 70.447 | 90.655 | 1.00 | 29.25 |
| ATOM | 1259 | CA  | TYR | 233 | 97.840  | 70.334 | 89.769 | 1.00 | 24.64 |
| ATOM | 1260 | CB  | TYR | 233 | 96.805  | 71.380 | 90.159 | 1.00 | 24.64 |
| ATOM | 1261 | CG  | TYR | 233 | 96.403  | 71.287 | 91.606 | 1.00 | 20.42 |
| ATOM | 1262 | CD1 | TYR | 233 | 95.511  | 70.312 | 92.036 | 1.00 | 16.93 |
| ATOM | 1263 | CE1 | TYR | 233 | 95.139  | 70.222 | 93.369 | 1.00 | 20.69 |
| ATOM | 1264 | CD2 | TYR | 233 | 96.922  | 72.170 | 92.546 | 1.00 | 20.67 |
| ATOM | 1265 | CE2 | TYR | 233 | 96.557  | 72.090 | 93.883 | 1.00 | 22.46 |
| ATOM | 1266 | CZ  | TYR | 233 | 95.666  | 71.114 | 94.289 | 1.00 | 22.03 |
| ATOM | 1267 | OH  | TYR | 233 | 95.295  | 71.040 | 95.613 | 1.00 | 25.90 |
| ATOM | 1268 | C   | TYR | 233 | 98.167  | 70.449 | 88.291 | 1.00 | 22.35 |
| ATOM | 1269 | O   | TYR | 233 | 97.996  | 71.513 | 87.688 | 1.00 | 22.95 |
| ATOM | 1270 | N   | PRO | 234 | 98.560  | 69.327 | 87.668 | 1.00 | 19.57 |
| ATOM | 1271 | CD  | PRO | 234 | 98.710  | 68.020 | 88.321 | 1.00 | 15.74 |
| ATOM | 1272 | CA  | PRO | 234 | 98.922  | 69.225 | 86.252 | 1.00 | 19.92 |
| ATOM | 1273 | CB  | PRO | 234 | 99.379  | 67.778 | 86.122 | 1.00 | 15.39 |

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FIGURE 1 (CONT.)

|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 1274 | CG  | PRO | 234 | 98.606  | 67.085 | 87.162 | 1.00 | 14.18 |
| ATOM | 1275 | C   | PRO | 234 | 97.812  | 69.535 | 85.266 | 1.00 | 21.74 |
| ATOM | 1276 | O   | PRO | 234 | 98.083  | 69.768 | 84.091 | 1.00 | 23.45 |
| ATOM | 1277 | N   | LEU | 235 | 96.568  | 69.527 | 85.734 | 1.00 | 23.76 |
| ATOM | 1278 | CA  | LEU | 235 | 95.436  | 69.806 | 84.856 | 1.00 | 24.11 |
| ATOM | 1279 | CB  | LEU | 235 | 94.316  | 68.800 | 85.100 | 1.00 | 22.93 |
| ATOM | 1280 | CG  | LEU | 235 | 94.640  | 67.346 | 84.788 | 1.00 | 17.74 |
| ATOM | 1281 | CD1 | LEU | 235 | 93.410  | 66.496 | 85.050 | 1.00 | 19.65 |
| ATOM | 1282 | CD2 | LEU | 235 | 95.074  | 67.241 | 83.346 | 1.00 | 15.28 |
| ATOM | 1283 | C   | LEU | 235 | 94.885  | 71.210 | 85.019 | 1.00 | 24.65 |
| ATOM | 1284 | O   | LEU | 235 | 93.947  | 71.597 | 84.315 | 1.00 | 26.71 |
| ATOM | 1285 | N   | ALA | 236 | 95.476  | 71.967 | 85.939 | 1.00 | 24.68 |
| ATOM | 1286 | CA  | ALA | 236 | 95.048  | 73.335 | 86.237 | 1.00 | 24.91 |
| ATOM | 1287 | CB  | ALA | 236 | 96.086  | 74.025 | 87.114 | 1.00 | 26.10 |
| ATOM | 1288 | C   | ALA | 236 | 94.718  | 74.215 | 85.031 | 1.00 | 24.07 |
| ATOM | 1289 | O   | ALA | 236 | 95.522  | 74.358 | 84.107 | 1.00 | 24.73 |
| ATOM | 1290 | N   | SER | 237 | 93.517  | 74.783 | 85.041 | 1.00 | 24.63 |
| ATOM | 1291 | CA  | SER | 237 | 93.070  | 75.678 | 83.981 | 1.00 | 25.43 |
| ATOM | 1292 | CB  | SER | 237 | 91.541  | 75.717 | 83.941 | 1.00 | 25.49 |
| ATOM | 1293 | OG  | SER | 237 | 91.009  | 74.422 | 83.729 | 1.00 | 26.13 |
| ATOM | 1294 | C   | SER | 237 | 93.625  | 77.068 | 84.292 | 1.00 | 25.26 |
| ATOM | 1295 | O   | SER | 237 | 93.017  | 77.826 | 85.050 | 1.00 | 24.30 |
| ATOM | 1296 | N   | LYS | 238 | 94.814  | 77.357 | 83.755 | 1.00 | 27.02 |
| ATOM | 1297 | CA  | LYS | 238 | 95.514  | 78.632 | 83.956 | 1.00 | 26.84 |
| ATOM | 1298 | CB  | LYS | 238 | 96.955  | 78.373 | 84.417 | 1.00 | 25.90 |
| ATOM | 1299 | CG  | LYS | 238 | 97.069  | 77.574 | 85.713 | 1.00 | 30.34 |
| ATOM | 1300 | CD  | LYS | 238 | 98.498  | 77.545 | 86.261 | 1.00 | 36.02 |
| ATOM | 1301 | CE  | LYS | 238 | 99.468  | 76.751 | 85.383 | 1.00 | 40.96 |
| ATOM | 1302 | NZ  | LYS | 238 | 99.312  | 75.265 | 85.478 | 1.00 | 43.36 |
| ATOM | 1303 | C   | LYS | 238 | 95.549  | 79.487 | 82.688 | 1.00 | 27.11 |
| ATOM | 1304 | O   | LYS | 238 | 95.469  | 78.960 | 81.588 | 1.00 | 28.11 |
| ATOM | 1305 | N   | ASP | 239 | 95.647  | 80.805 | 82.839 | 1.00 | 27.73 |
| ATOM | 1306 | CA  | ASP | 239 | 95.712  | 81.703 | 81.684 | 1.00 | 28.78 |
| ATOM | 1307 | CB  | ASP | 239 | 95.005  | 83.044 | 81.968 | 1.00 | 26.56 |
| ATOM | 1308 | CG  | ASP | 239 | 95.633  | 83.832 | 83.116 | 1.00 | 24.59 |
| ATOM | 1309 | OD1 | ASP | 239 | 96.564  | 83.334 | 83.766 | 1.00 | 26.84 |
| ATOM | 1310 | OD2 | ASP | 239 | 95.189  | 84.968 | 83.374 | 1.00 | 24.38 |
| ATOM | 1311 | C   | ASP | 239 | 97.169  | 81.927 | 81.268 | 1.00 | 30.60 |
| ATOM | 1312 | O   | ASP | 239 | 98.087  | 81.343 | 81.855 | 1.00 | 32.51 |
| ATOM | 1313 | N   | ALA | 240 | 97.389  | 82.805 | 80.296 | 1.00 | 30.28 |
| ATOM | 1314 | CA  | ALA | 240 | 98.737  | 83.082 | 79.811 | 1.00 | 31.43 |
| ATOM | 1315 | CB  | ALA | 240 | 98.686  | 84.111 | 78.705 | 1.00 | 32.61 |
| ATOM | 1316 | C   | ALA | 240 | 99.701  | 83.536 | 80.905 | 1.00 | 33.16 |
| ATOM | 1317 | O   | ALA | 240 | 100.915 | 83.424 | 80.756 | 1.00 | 34.13 |
| ATOM | 1318 | N   | LYS | 241 | 99.158  | 84.024 | 82.013 | 1.00 | 34.52 |
| ATOM | 1319 | CA  | LYS | 241 | 99.985  | 84.507 | 83.114 | 1.00 | 34.81 |
| ATOM | 1320 | CB  | LYS | 241 | 99.422  | 85.834 | 83.639 | 1.00 | 37.50 |
| ATOM | 1321 | CG  | LYS | 241 | 98.935  | 86.783 | 82.540 | 1.00 | 43.35 |
| ATOM | 1322 | CD  | LYS | 241 | 100.062 | 87.283 | 81.631 | 1.00 | 46.22 |
| ATOM | 1323 | CE  | LYS | 241 | 100.841 | 88.420 | 82.278 | 1.00 | 48.19 |
| ATOM | 1324 | NZ  | LYS | 241 | 99.952  | 89.571 | 82.619 | 1.00 | 51.12 |
| ATOM | 1325 | C   | LYS | 241 | 100.105 | 83.498 | 84.257 | 1.00 | 33.59 |
| ATOM | 1326 | O   | LYS | 241 | 100.425 | 83.872 | 85.382 | 1.00 | 35.65 |
| ATOM | 1327 | N   | LYS | 242 | 99.834  | 82.229 | 83.967 | 1.00 | 31.55 |
| ATOM | 1328 | CA  | LYS | 242 | 99.909  | 81.160 | 84.963 | 1.00 | 30.28 |
| ATOM | 1329 | CB  | LYS | 242 | 101.349 | 80.959 | 85.434 | 1.00 | 32.09 |
| ATOM | 1330 | CG  | LYS | 242 | 102.261 | 80.473 | 84.336 | 1.00 | 39.25 |
| ATOM | 1331 | CD  | LYS | 242 | 101.699 | 79.221 | 83.672 | 1.00 | 46.14 |

FIGURE 1 (CONT.)

|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 1332 | CE  | LYS | 242 | 102.685 | 78.627 | 82.676 | 1.00 | 51.26 |
| ATOM | 1333 | NZ  | LYS | 242 | 103.060 | 79.601 | 81.608 | 1.00 | 54.72 |
| ATOM | 1334 | C   | LYS | 242 | 98.972  | 81.316 | 86.160 | 1.00 | 28.29 |
| ATOM | 1335 | O   | LYS | 242 | 99.236  | 80.787 | 87.249 | 1.00 | 26.69 |
| ATOM | 1336 | N   | GLN | 243 | 97.856  | 82.000 | 85.926 | 1.00 | 26.16 |
| ATOM | 1337 | CA  | GLN | 243 | 96.833  | 82.229 | 86.941 | 1.00 | 24.73 |
| ATOM | 1338 | CB  | GLN | 243 | 96.364  | 83.679 | 86.905 | 1.00 | 25.73 |
| ATOM | 1339 | CG  | GLN | 243 | 97.449  | 84.714 | 87.041 | 1.00 | 28.69 |
| ATOM | 1340 | CD  | GLN | 243 | 96.883  | 86.108 | 86.960 | 1.00 | 31.37 |
| ATOM | 1341 | OE1 | GLN | 243 | 97.213  | 86.874 | 86.062 | 1.00 | 35.38 |
| ATOM | 1342 | NE2 | GLN | 243 | 95.986  | 86.431 | 87.877 | 1.00 | 35.92 |
| ATOM | 1343 | C   | GLN | 243 | 95.625  | 81.346 | 86.646 | 1.00 | 23.19 |
| ATOM | 1344 | O   | GLN | 243 | 95.335  | 81.062 | 85.488 | 1.00 | 22.08 |
| ATOM | 1345 | N   | LEU | 244 | 94.907  | 80.934 | 87.684 | 1.00 | 22.67 |
| ATOM | 1346 | CA  | LEU | 244 | 93.723  | 80.111 | 87.484 | 1.00 | 23.46 |
| ATOM | 1347 | CB  | LEU | 244 | 93.144  | 79.655 | 88.824 | 1.00 | 22.03 |
| ATOM | 1348 | CG  | LEU | 244 | 93.986  | 78.729 | 89.695 | 1.00 | 18.65 |
| ATOM | 1349 | CD1 | LEU | 244 | 93.196  | 78.359 | 90.934 | 1.00 | 13.02 |
| ATOM | 1350 | CD2 | LEU | 244 | 94.361  | 77.478 | 88.913 | 1.00 | 18.74 |
| ATOM | 1351 | C   | LEU | 244 | 92.690  | 80.959 | 86.757 | 1.00 | 23.82 |
| ATOM | 1352 | O   | LEU | 244 | 92.302  | 82.018 | 87.245 | 1.00 | 25.78 |
| ATOM | 1353 | N   | LEU | 245 | 92.279  | 80.531 | 85.569 | 1.00 | 24.26 |
| ATOM | 1354 | CA  | LEU | 245 | 91.286  | 81.298 | 84.836 | 1.00 | 22.59 |
| ATOM | 1355 | CB  | LEU | 245 | 91.181  | 80.843 | 83.372 | 1.00 | 24.90 |
| ATOM | 1356 | CG  | LEU | 245 | 91.196  | 79.370 | 82.962 | 1.00 | 25.75 |
| ATOM | 1357 | CD1 | LEU | 245 | 90.061  | 78.644 | 83.632 | 1.00 | 27.83 |
| ATOM | 1358 | CD2 | LEU | 245 | 91.086  | 79.250 | 81.443 | 1.00 | 21.78 |
| ATOM | 1359 | C   | LEU | 245 | 89.949  | 81.241 | 85.564 | 1.00 | 21.43 |
| ATOM | 1360 | O   | LEU | 245 | 89.665  | 80.286 | 86.286 | 1.00 | 22.49 |
| ATOM | 1361 | N   | CYS | 246 | 89.151  | 82.288 | 85.401 | 1.00 | 20.00 |
| ATOM | 1362 | CA  | CYS | 246 | 87.858  | 82.388 | 86.057 | 1.00 | 18.86 |
| ATOM | 1363 | CB  | CYS | 246 | 88.004  | 83.243 | 87.321 | 1.00 | 17.47 |
| ATOM | 1364 | SG  | CYS | 246 | 86.569  | 83.374 | 88.399 | 1.00 | 17.81 |
| ATOM | 1365 | C   | CYS | 246 | 86.852  | 83.027 | 85.106 | 1.00 | 20.06 |
| ATOM | 1366 | O   | CYS | 246 | 87.217  | 83.804 | 84.216 | 1.00 | 18.69 |
| ATOM | 1367 | N   | GLY | 247 | 85.592  | 82.646 | 85.265 | 1.00 | 19.49 |
| ATOM | 1368 | CA  | GLY | 247 | 84.532  | 83.197 | 84.449 | 1.00 | 17.64 |
| ATOM | 1369 | C   | GLY | 247 | 83.474  | 83.715 | 85.398 | 1.00 | 16.99 |
| ATOM | 1370 | O   | GLY | 247 | 83.420  | 83.287 | 86.553 | 1.00 | 18.25 |
| ATOM | 1371 | N   | ALA | 248 | 82.630  | 81.626 | 84.935 | 1.00 | 16.02 |
| ATOM | 1372 | CA  | ALA | 248 | 81.595  | 85.189 | 85.792 | 1.00 | 15.37 |
| ATOM | 1373 | CB  | ALA | 248 | 82.055  | 86.520 | 86.362 | 1.00 | 10.50 |
| ATOM | 1374 | C   | ALA | 248 | 80.299  | 85.360 | 85.016 | 1.00 | 15.60 |
| ATOM | 1375 | O   | ALA | 248 | 80.319  | 85.477 | 83.788 | 1.00 | 15.68 |
| ATOM | 1376 | N   | ALA | 249 | 79.174  | 85.357 | 85.724 | 1.00 | 15.70 |
| ATOM | 1377 | CA  | ALA | 249 | 77.874  | 85.512 | 85.077 | 1.00 | 15.74 |
| ATOM | 1378 | CB  | ALA | 249 | 76.918  | 84.445 | 85.574 | 1.00 | 12.70 |
| ATOM | 1379 | C   | ALA | 249 | 77.282  | 86.891 | 85.327 | 1.00 | 14.03 |
| ATOM | 1380 | O   | ALA | 249 | 77.329  | 87.381 | 86.452 | 1.00 | 14.73 |
| ATOM | 1381 | N   | ILE | 250 | 76.759  | 87.531 | 84.286 | 1.00 | 12.46 |
| ATOM | 1382 | CA  | ILE | 250 | 76.123  | 88.835 | 84.445 | 1.00 | 14.51 |
| ATOM | 1383 | CB  | ILE | 250 | 76.965  | 90.018 | 83.895 | 1.00 | 11.80 |
| ATOM | 1384 | CG2 | ILE | 250 | 78.249  | 90.162 | 84.659 | 1.00 | 9.96  |
| ATOM | 1385 | CG1 | ILE | 250 | 77.207  | 89.866 | 82.395 | 1.00 | 15.67 |
| ATOM | 1386 | CD1 | ILE | 250 | 77.623  | 91.154 | 81.705 | 1.00 | 17.25 |
| ATOM | 1387 | C   | ILE | 250 | 74.772  | 88.844 | 83.739 | 1.00 | 17.19 |
| ATOM | 1388 | O   | ILE | 250 | 74.460  | 87.948 | 82.959 | 1.00 | 18.56 |
| ATOM | 1389 | N   | GLY | 251 | 73.950  | 89.828 | 84.074 | 1.00 | 18.09 |



FIGURE 1 (CONT.)

|      |      |     |     |     |        |         |        |      |       |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 1390 | CA  | GLY | 251 | 72.655 | 89.954  | 83.447 | 1.00 | 18.30 |
| ATOM | 1391 | C   | GLY | 251 | 72.821 | 90.758  | 82.176 | 1.00 | 20.39 |
| ATOM | 1392 | O   | GLY | 251 | 73.944 | 90.968  | 81.721 | 1.00 | 20.47 |
| ATOM | 1393 | N   | THR | 252 | 71.715 | 91.265  | 81.642 | 1.00 | 23.81 |
| ATOM | 1394 | CA  | THR | 252 | 71.740 | 92.036  | 80.405 | 1.00 | 26.27 |
| ATOM | 1395 | CB  | THR | 252 | 70.961 | 91.309  | 79.288 | 1.00 | 24.89 |
| ATOM | 1396 | OG1 | THR | 252 | 69.704 | 90.844  | 79.803 | 1.00 | 27.82 |
| ATOM | 1397 | CG2 | THR | 252 | 71.764 | 90.127  | 78.757 | 1.00 | 21.50 |
| ATOM | 1398 | C   | THR | 252 | 71.216 | 93.467  | 80.537 | 1.00 | 28.88 |
| ATOM | 1399 | O   | THR | 252 | 71.085 | 94.182  | 79.540 | 1.00 | 30.63 |
| ATOM | 1400 | N   | HIS | 253 | 70.875 | 93.877  | 81.753 | 1.00 | 29.72 |
| ATOM | 1401 | CA  | HIS | 253 | 70.393 | 95.235  | 81.970 | 1.00 | 32.38 |
| ATOM | 1402 | CB  | HIS | 253 | 69.719 | 95.350  | 83.335 | 1.00 | 35.13 |
| ATOM | 1403 | CG  | HIS | 253 | 68.545 | 94.438  | 83.516 | 1.00 | 38.59 |
| ATOM | 1404 | CD2 | HIS | 253 | 67.485 | 94.186  | 82.710 | 1.00 | 40.91 |
| ATOM | 1405 | ND1 | HIS | 253 | 68.367 | 93.659  | 84.636 | 1.00 | 41.86 |
| ATOM | 1406 | CE1 | HIS | 253 | 67.251 | 92.968  | 84.521 | 1.00 | 42.51 |
| ATOM | 1407 | NE2 | HIS | 253 | 66.691 | 93.269  | 83.360 | 1.00 | 43.09 |
| ATOM | 1408 | C   | HIS | 253 | 71.596 | 96.171  | 81.905 | 1.00 | 34.27 |
| ATOM | 1409 | O   | HIS | 253 | 72.735 | 95.728  | 82.055 | 1.00 | 34.56 |
| ATOM | 1410 | N   | GLU | 254 | 71.347 | 97.461  | 81.696 | 1.00 | 36.70 |
| ATOM | 1411 | CA  | GLU | 254 | 72.415 | 98.467  | 81.621 | 1.00 | 38.22 |
| ATOM | 1412 | CB  | GLU | 254 | 71.811 | 99.877  | 81.566 | 1.00 | 39.91 |
| ATOM | 1413 | CG  | GLU | 254 | 70.970 | 100.167 | 80.331 | 1.00 | 44.25 |
| ATOM | 1414 | CD  | GLU | 254 | 71.797 | 100.264 | 79.060 | 1.00 | 47.81 |
| ATOM | 1415 | OE1 | GLU | 254 | 72.924 | 100.809 | 79.126 | 1.00 | 49.46 |
| ATOM | 1416 | OE2 | GLU | 254 | 71.316 | 99.808  | 77.995 | 1.00 | 46.89 |
| ATOM | 1417 | C   | GLU | 254 | 73.363 | 98.376  | 82.821 | 1.00 | 38.45 |
| ATOM | 1418 | O   | GLU | 254 | 74.576 | 98.556  | 82.690 | 1.00 | 37.95 |
| ATOM | 1419 | N   | ASP | 255 | 72.791 | 98.085  | 83.986 | 1.00 | 39.23 |
| ATOM | 1420 | CA  | ASP | 255 | 73.537 | 97.960  | 85.238 | 1.00 | 40.62 |
| ATOM | 1421 | CB  | ASP | 255 | 72.618 | 97.427  | 86.346 | 1.00 | 48.75 |
| ATOM | 1422 | CG  | ASP | 255 | 71.337 | 98.236  | 86.500 | 1.00 | 59.02 |
| ATOM | 1423 | OD1 | ASP | 255 | 71.359 | 99.251  | 87.238 | 1.00 | 63.37 |
| ATOM | 1424 | OD2 | ASP | 255 | 70.306 | 97.841  | 85.898 | 1.00 | 63.08 |
| ATOM | 1425 | C   | ASP | 255 | 74.698 | 96.985  | 85.080 | 1.00 | 38.56 |
| ATOM | 1426 | O   | ASP | 255 | 75.763 | 97.140  | 85.687 | 1.00 | 37.91 |
| ATOM | 1427 | N   | ASP | 256 | 74.472 | 95.972  | 84.255 | 1.00 | 36.23 |
| ATOM | 1428 | CA  | ASP | 256 | 75.467 | 94.943  | 84.028 | 1.00 | 32.80 |
| ATOM | 1429 | CB  | ASP | 256 | 74.831 | 93.752  | 83.324 | 1.00 | 31.43 |
| ATOM | 1430 | CG  | ASP | 256 | 73.752 | 93.113  | 84.164 | 1.00 | 31.85 |
| ATOM | 1431 | OD1 | ASP | 256 | 74.088 | 92.491  | 85.193 | 1.00 | 32.92 |
| ATOM | 1432 | OD2 | ASP | 256 | 72.566 | 93.253  | 83.817 | 1.00 | 33.76 |
| ATOM | 1433 | C   | ASP | 256 | 76.702 | 95.433  | 83.311 | 1.00 | 30.28 |
| ATOM | 1434 | O   | ASP | 256 | 77.730 | 94.760  | 83.307 | 1.00 | 30.73 |
| ATOM | 1435 | N   | LYS | 257 | 76.623 | 96.620  | 82.732 | 1.00 | 27.82 |
| ATOM | 1436 | CA  | LYS | 257 | 77.778 | 97.172  | 82.054 | 1.00 | 26.56 |
| ATOM | 1437 | CB  | LYS | 257 | 77.360 | 98.332  | 81.163 | 1.00 | 27.33 |
| ATOM | 1438 | CG  | LYS | 257 | 76.374 | 97.918  | 80.089 | 1.00 | 27.87 |
| ATOM | 1439 | CD  | LYS | 257 | 76.064 | 99.065  | 79.168 | 1.00 | 29.75 |
| ATOM | 1440 | CE  | LYS | 257 | 75.247 | 98.598  | 77.987 | 1.00 | 31.51 |
| ATOM | 1441 | NZ  | LYS | 257 | 75.030 | 99.713  | 77.033 | 1.00 | 33.96 |
| ATOM | 1442 | C   | LYS | 257 | 78.806 | 97.605  | 83.104 | 1.00 | 25.35 |
| ATOM | 1443 | O   | LYS | 257 | 80.003 | 97.327  | 82.962 | 1.00 | 26.37 |
| ATOM | 1444 | N   | TYR | 258 | 78.321 | 98.211  | 84.189 | 1.00 | 23.85 |
| ATOM | 1445 | CA  | TYR | 258 | 79.171 | 98.661  | 85.294 | 1.00 | 22.66 |
| ATOM | 1446 | CB  | TYR | 258 | 78.346 | 99.474  | 86.308 | 1.00 | 18.97 |
| ATOM | 1447 | CG  | TYR | 258 | 78.981 | 99.660  | 87.677 | 1.00 | 18.12 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |         |        |      |       |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 1448 | CD1 | TYR | 258 | 80.182 | 100.357 | 87.832 | 1.00 | 19.37 |
| ATOM | 1449 | CE1 | TYR | 258 | 80.765 | 100.518 | 89.096 | 1.00 | 19.31 |
| ATOM | 1450 | CD2 | TYR | 258 | 78.380 | 99.129  | 88.820 | 1.00 | 17.20 |
| ATOM | 1451 | CE2 | TYR | 258 | 78.955 | 99.284  | 90.081 | 1.00 | 17.71 |
| ATOM | 1452 | CZ  | TYR | 258 | 80.144 | 99.978  | 90.213 | 1.00 | 18.86 |
| ATOM | 1453 | OH  | TYR | 258 | 80.711 | 100.126 | 91.460 | 1.00 | 23.15 |
| ATOM | 1454 | C   | TYR | 258 | 79.803 | 97.440  | 85.960 | 1.00 | 23.75 |
| ATOM | 1455 | O   | TYR | 258 | 81.028 | 97.365  | 86.127 | 1.00 | 26.26 |
| ATOM | 1456 | N   | ARG | 259 | 78.959 | 96.487  | 86.335 | 1.00 | 22.76 |
| ATOM | 1457 | CA  | ARG | 259 | 79.415 | 95.251  | 86.955 | 1.00 | 21.36 |
| ATOM | 1458 | CB  | ARG | 259 | 78.231 | 94.307  | 87.120 | 1.00 | 21.72 |
| ATOM | 1459 | CG  | ARG | 259 | 78.579 | 92.912  | 87.567 | 1.00 | 20.25 |
| ATOM | 1460 | CD  | ARG | 259 | 77.328 | 92.068  | 87.586 | 1.00 | 16.94 |
| ATOM | 1461 | NE  | ARG | 259 | 76.371 | 92.538  | 88.583 | 1.00 | 9.97  |
| ATOM | 1462 | CZ  | ARG | 259 | 76.422 | 92.204  | 89.866 | 1.00 | 11.33 |
| ATOM | 1463 | NH1 | ARG | 259 | 77.381 | 91.403  | 90.305 | 1.00 | 15.57 |
| ATOM | 1464 | NH2 | ARG | 259 | 75.511 | 92.658  | 90.710 | 1.00 | 9.18  |
| ATOM | 1465 | C   | ARG | 259 | 80.479 | 94.607  | 86.070 | 1.00 | 20.76 |
| ATOM | 1466 | O   | ARG | 259 | 81.534 | 94.217  | 86.555 | 1.00 | 23.26 |
| ATOM | 1467 | N   | LEU | 260 | 80.217 | 94.557  | 84.766 | 1.00 | 19.61 |
| ATOM | 1468 | CA  | LEU | 260 | 81.149 | 93.986  | 83.800 | 1.00 | 19.57 |
| ATOM | 1469 | CB  | LEU | 260 | 80.614 | 94.141  | 82.372 | 1.00 | 15.34 |
| ATOM | 1470 | CG  | LEU | 260 | 81.576 | 93.695  | 81.270 | 1.00 | 12.31 |
| ATOM | 1471 | CD1 | LEU | 260 | 81.799 | 92.187  | 81.352 | 1.00 | 13.03 |
| ATOM | 1472 | CD2 | LEU | 260 | 81.035 | 94.079  | 79.914 | 1.00 | 11.42 |
| ATOM | 1473 | C   | LEU | 260 | 82.496 | 94.684  | 83.898 | 1.00 | 22.22 |
| ATOM | 1474 | O   | LEU | 260 | 83.549 | 94.038  | 83.867 | 1.00 | 22.00 |
| ATOM | 1475 | N   | ASP | 261 | 82.462 | 96.008  | 83.997 | 1.00 | 24.36 |
| ATOM | 1476 | CA  | ASP | 261 | 83.688 | 96.785  | 84.090 | 1.00 | 23.45 |
| ATOM | 1477 | CB  | ASP | 261 | 83.389 | 98.284  | 84.092 | 1.00 | 24.33 |
| ATOM | 1478 | CG  | ASP | 261 | 82.896 | 98.788  | 82.739 | 1.00 | 26.27 |
| ATOM | 1479 | OD1 | ASP | 261 | 83.111 | 98.103  | 81.719 | 1.00 | 19.29 |
| ATOM | 1480 | OD2 | ASP | 261 | 82.295 | 99.881  | 82.693 | 1.00 | 32.41 |
| ATOM | 1481 | C   | ASP | 261 | 84.480 | 96.378  | 85.315 | 1.00 | 22.43 |
| ATOM | 1482 | O   | ASP | 261 | 85.689 | 96.169  | 85.219 | 1.00 | 25.11 |
| ATOM | 1483 | N   | LEU | 262 | 83.801 | 96.197  | 86.445 | 1.00 | 19.65 |
| ATOM | 1484 | CA  | LEU | 262 | 84.482 | 95.782  | 87.670 | 1.00 | 18.60 |
| ATOM | 1485 | CB  | LEU | 262 | 83.547 | 95.857  | 88.877 | 1.00 | 16.65 |
| ATOM | 1486 | CG  | LEU | 262 | 82.947 | 97.231  | 89.194 | 1.00 | 18.61 |
| ATOM | 1487 | CD1 | LEU | 262 | 82.651 | 97.321  | 90.682 | 1.00 | 14.11 |
| ATOM | 1488 | CD2 | LEU | 262 | 83.910 | 98.341  | 88.782 | 1.00 | 16.63 |
| ATOM | 1489 | C   | LEU | 262 | 85.030 | 94.368  | 87.522 | 1.00 | 19.71 |
| ATOM | 1490 | O   | LEU | 262 | 86.100 | 94.044  | 88.050 | 1.00 | 20.31 |
| ATOM | 1491 | N   | LEU | 263 | 84.306 | 93.533  | 86.782 | 1.00 | 19.72 |
| ATOM | 1492 | CA  | LEU | 263 | 84.728 | 92.158  | 86.546 | 1.00 | 18.62 |
| ATOM | 1493 | CB  | LEU | 263 | 83.581 | 91.321  | 85.970 | 1.00 | 15.30 |
| ATOM | 1494 | CG  | LEU | 263 | 82.386 | 91.120  | 86.909 | 1.00 | 13.44 |
| ATOM | 1495 | CD1 | LEU | 263 | 81.319 | 90.307  | 86.215 | 1.00 | 12.65 |
| ATOM | 1496 | CD2 | LEU | 263 | 82.828 | 90.450  | 88.194 | 1.00 | 8.53  |
| ATOM | 1497 | C   | LEU | 263 | 85.925 | 92.145  | 85.608 | 1.00 | 19.87 |
| ATOM | 1498 | O   | LEU | 263 | 86.802 | 91.288  | 85.730 | 1.00 | 19.89 |
| ATOM | 1499 | N   | ALA | 264 | 85.966 | 93.104  | 84.685 | 1.00 | 20.77 |
| ATOM | 1500 | CA  | ALA | 264 | 87.079 | 93.220  | 83.741 | 1.00 | 21.02 |
| ATOM | 1501 | CB  | ALA | 264 | 86.809 | 94.324  | 82.728 | 1.00 | 19.62 |
| ATOM | 1502 | C   | ALA | 264 | 88.331 | 93.540  | 84.553 | 1.00 | 20.05 |
| ATOM | 1503 | O   | ALA | 264 | 89.330 | 92.824  | 84.484 | 1.00 | 19.96 |
| ATOM | 1504 | N   | LEU | 265 | 88.235 | 94.582  | 85.374 | 1.00 | 19.65 |
| ATOM | 1505 | CA  | LEU | 265 | 89.326 | 95.002  | 86.240 | 1.00 | 17.63 |

1448 1449 1450 1451 1452 1453 1454 1455 1456 1457 1458 1459 1460 1461 1462 1463 1464 1465 1466 1467 1468 1469 1470 1471 1472 1473 1474 1475 1476 1477 1478 1479 1480 1481 1482 1483 1484 1485 1486 1487 1488 1489 1490 1491 1492 1493 1494 1495 1496 1497 1498 1499 1500 1501 1502 1503 1504 1505

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1506 | CB  | LEU | 265 | 88.875 | 96.165 | 87.118 | 1.00 | 14.88 |
| ATOM | 1507 | CG  | LEU | 265 | 88.827 | 97.558 | 86.487 | 1.00 | 16.17 |
| ATOM | 1508 | CD1 | LEU | 265 | 88.122 | 98.539 | 87.420 | 1.00 | 14.22 |
| ATOM | 1509 | CD2 | LEU | 265 | 90.236 | 98.024 | 86.198 | 1.00 | 9.91  |
| ATOM | 1510 | C   | LEU | 265 | 89.781 | 93.856 | 87.136 | 1.00 | 19.52 |
| ATOM | 1511 | O   | LEU | 265 | 90.945 | 93.792 | 87.517 | 1.00 | 23.94 |
| ATOM | 1512 | N   | ALA | 266 | 88.851 | 92.975 | 87.495 | 1.00 | 17.94 |
| ATOM | 1513 | CA  | ALA | 266 | 89.144 | 91.827 | 88.349 | 1.00 | 14.70 |
| ATOM | 1514 | CB  | ALA | 266 | 87.852 | 91.215 | 88.859 | 1.00 | 14.20 |
| ATOM | 1515 | C   | ALA | 266 | 89.956 | 90.776 | 87.605 | 1.00 | 14.73 |
| ATOM | 1516 | O   | ALA | 266 | 90.602 | 89.925 | 88.219 | 1.00 | 14.46 |
| ATOM | 1517 | N   | GLY | 267 | 89.901 | 90.825 | 86.280 | 1.00 | 14.47 |
| ATOM | 1518 | CA  | GLY | 267 | 90.638 | 89.869 | 85.480 | 1.00 | 15.93 |
| ATOM | 1519 | C   | GLY | 267 | 89.848 | 88.638 | 85.089 | 1.00 | 19.86 |
| ATOM | 1520 | O   | GLY | 267 | 90.427 | 87.567 | 84.889 | 1.00 | 23.99 |
| ATOM | 1521 | N   | VAL | 268 | 88.528 | 88.774 | 84.996 | 1.00 | 21.02 |
| ATOM | 1522 | CA  | VAL | 268 | 87.660 | 87.670 | 84.607 | 1.00 | 19.03 |
| ATOM | 1523 | CB  | VAL | 268 | 86.178 | 88.107 | 84.620 | 1.00 | 16.96 |
| ATOM | 1524 | CG1 | VAL | 268 | 85.891 | 89.056 | 83.477 | 1.00 | 13.08 |
| ATOM | 1525 | CG2 | VAL | 268 | 85.266 | 86.907 | 84.565 | 1.00 | 18.26 |
| ATOM | 1526 | C   | VAL | 268 | 88.076 | 87.274 | 83.188 | 1.00 | 19.74 |
| ATOM | 1527 | O   | VAL | 268 | 88.452 | 88.136 | 82.393 | 1.00 | 21.80 |
| ATOM | 1528 | N   | ASP | 269 | 88.035 | 85.980 | 82.886 | 1.00 | 18.77 |
| ATOM | 1529 | CA  | ASP | 269 | 88.428 | 85.481 | 81.571 | 1.00 | 15.89 |
| ATOM | 1530 | CB  | ASP | 269 | 89.229 | 84.193 | 81.728 | 1.00 | 15.41 |
| ATOM | 1531 | CG  | ASP | 269 | 90.448 | 84.371 | 82.604 | 1.00 | 19.66 |
| ATOM | 1532 | OD1 | ASP | 269 | 91.555 | 84.564 | 82.070 | 1.00 | 22.69 |
| ATOM | 1533 | OD2 | ASP | 269 | 90.303 | 84.319 | 83.835 | 1.00 | 22.25 |
| ATOM | 1534 | C   | ASP | 269 | 87.273 | 85.245 | 80.597 | 1.00 | 16.00 |
| ATOM | 1535 | O   | ASP | 269 | 87.419 | 85.442 | 79.386 | 1.00 | 17.09 |
| ATOM | 1536 | N   | VAL | 270 | 86.146 | 84.770 | 81.115 | 1.00 | 16.22 |
| ATOM | 1537 | CA  | VAL | 270 | 84.978 | 84.491 | 80.289 | 1.00 | 16.09 |
| ATOM | 1538 | CB  | VAL | 270 | 84.782 | 82.974 | 80.021 | 1.00 | 15.10 |
| ATOM | 1539 | CG1 | VAL | 270 | 85.722 | 82.506 | 78.967 | 1.00 | 20.52 |
| ATOM | 1540 | CG2 | VAL | 270 | 85.024 | 82.174 | 81.275 | 1.00 | 15.72 |
| ATOM | 1541 | C   | VAL | 270 | 83.759 | 84.976 | 81.024 | 1.00 | 16.90 |
| ATOM | 1542 | O   | VAL | 270 | 83.689 | 84.857 | 82.248 | 1.00 | 18.88 |
| ATOM | 1543 | N   | VAL | 271 | 82.797 | 85.512 | 80.284 | 1.00 | 15.33 |
| ATOM | 1544 | CA  | VAL | 271 | 81.574 | 86.005 | 80.885 | 1.00 | 13.74 |
| ATOM | 1545 | CB  | VAL | 271 | 81.528 | 87.542 | 80.857 | 1.00 | 11.48 |
| ATOM | 1546 | CG1 | VAL | 271 | 80.130 | 88.035 | 81.173 | 1.00 | 11.74 |
| ATOM | 1547 | CG2 | VAL | 271 | 82.497 | 88.096 | 81.881 | 1.00 | 11.95 |
| ATOM | 1548 | C   | VAL | 271 | 80.333 | 85.420 | 80.215 | 1.00 | 14.45 |
| ATOM | 1549 | O   | VAL | 271 | 80.222 | 85.401 | 78.986 | 1.00 | 15.35 |
| ATOM | 1550 | N   | VAL | 272 | 79.421 | 84.904 | 81.028 | 1.00 | 13.08 |
| ATOM | 1551 | CA  | VAL | 272 | 78.193 | 84.341 | 80.511 | 1.00 | 12.88 |
| ATOM | 1552 | CB  | VAL | 272 | 77.924 | 82.906 | 81.050 | 1.00 | 11.78 |
| ATOM | 1553 | CG1 | VAL | 272 | 77.855 | 82.893 | 82.547 | 1.00 | 13.59 |
| ATOM | 1554 | CG2 | VAL | 272 | 76.630 | 82.371 | 80.485 | 1.00 | 11.58 |
| ATOM | 1555 | C   | VAL | 272 | 77.020 | 85.255 | 80.843 | 1.00 | 14.54 |
| ATOM | 1556 | O   | VAL | 272 | 76.896 | 85.751 | 81.971 | 1.00 | 14.50 |
| ATOM | 1557 | N   | LEU | 273 | 76.215 | 85.535 | 79.823 | 1.00 | 14.49 |
| ATOM | 1558 | CA  | LEU | 273 | 75.031 | 86.362 | 79.969 | 1.00 | 13.78 |
| ATOM | 1559 | CB  | LEU | 273 | 74.703 | 87.005 | 78.628 | 1.00 | 10.64 |
| ATOM | 1560 | CG  | LEU | 273 | 75.900 | 87.845 | 78.168 | 1.00 | 8.78  |
| ATOM | 1561 | CD1 | LEU | 273 | 75.649 | 88.474 | 76.836 | 1.00 | 10.66 |
| ATOM | 1562 | CD2 | LEU | 273 | 76.186 | 88.927 | 79.188 | 1.00 | 9.83  |
| ATOM | 1563 | C   | LEU | 273 | 73.916 | 85.434 | 80.469 | 1.00 | 16.26 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1564 | O   | LEU | 273 | 73.510 | 84.478 | 79.781 | 1.00 | 15.19 |
| ATOM | 1565 | N   | ASP | 274 | 73.499 | 85.689 | 81.708 | 1.00 | 15.97 |
| ATOM | 1566 | CA  | ASP | 274 | 72.492 | 84.910 | 82.430 | 1.00 | 14.76 |
| ATOM | 1567 | CB  | ASP | 274 | 72.706 | 85.144 | 83.932 | 1.00 | 14.18 |
| ATOM | 1568 | CG  | ASP | 274 | 72.150 | 84.036 | 84.789 | 1.00 | 18.31 |
| ATOM | 1569 | OD1 | ASP | 274 | 72.007 | 82.901 | 84.291 | 1.00 | 23.20 |
| ATOM | 1570 | OD2 | ASP | 274 | 71.882 | 84.294 | 85.985 | 1.00 | 21.30 |
| ATOM | 1571 | C   | ASP | 274 | 71.028 | 85.177 | 82.066 | 1.00 | 13.69 |
| ATOM | 1572 | O   | ASP | 274 | 70.494 | 86.253 | 82.339 | 1.00 | 16.74 |
| ATOM | 1573 | N   | SER | 275 | 70.367 | 84.174 | 81.501 | 1.00 | 11.17 |
| ATOM | 1574 | CA  | SER | 275 | 68.963 | 84.287 | 81.122 | 1.00 | 10.14 |
| ATOM | 1575 | CB  | SER | 275 | 68.784 | 85.240 | 79.934 | 1.00 | 8.75  |
| ATOM | 1576 | OG  | SER | 275 | 69.604 | 84.882 | 78.828 | 1.00 | 18.88 |
| ATOM | 1577 | C   | SER | 275 | 68.344 | 82.937 | 80.802 | 1.00 | 10.53 |
| ATOM | 1578 | O   | SER | 275 | 69.030 | 82.021 | 80.351 | 1.00 | 10.72 |
| ATOM | 1579 | N   | SER | 276 | 67.054 | 82.810 | 81.092 | 1.00 | 12.08 |
| ATOM | 1580 | CA  | SER | 276 | 66.311 | 81.589 | 80.835 | 1.00 | 11.23 |
| ATOM | 1581 | CB  | SER | 276 | 65.058 | 81.558 | 81.702 | 1.00 | 7.13  |
| ATOM | 1582 | OG  | SER | 276 | 64.208 | 82.626 | 81.348 | 1.00 | 7.88  |
| ATOM | 1583 | C   | SER | 276 | 65.921 | 81.513 | 79.359 | 1.00 | 13.13 |
| ATOM | 1584 | O   | SER | 276 | 65.594 | 80.439 | 78.845 | 1.00 | 17.69 |
| ATOM | 1585 | N   | GLN | 277 | 65.930 | 82.657 | 78.687 | 1.00 | 12.48 |
| ATOM | 1586 | CA  | GLN | 277 | 65.583 | 82.720 | 77.275 | 1.00 | 14.28 |
| ATOM | 1587 | CB  | GLN | 277 | 64.093 | 83.058 | 77.115 | 1.00 | 13.50 |
| ATOM | 1588 | CG  | GLN | 277 | 63.387 | 82.326 | 75.968 | 1.00 | 10.64 |
| ATOM | 1589 | CD  | GLN | 277 | 63.715 | 82.880 | 74.584 | 1.00 | 13.67 |
| ATOM | 1590 | OE1 | GLN | 277 | 62.891 | 83.547 | 73.959 | 1.00 | 13.62 |
| ATOM | 1591 | NE2 | GLN | 277 | 64.906 | 82.574 | 74.088 | 1.00 | 14.26 |
| ATOM | 1592 | C   | GLN | 277 | 66.463 | 83.823 | 76.702 | 1.00 | 15.33 |
| ATOM | 1593 | O   | GLN | 277 | 66.047 | 84.981 | 76.612 | 1.00 | 17.75 |
| ATOM | 1594 | N   | GLY | 278 | 67.685 | 83.453 | 76.329 | 1.00 | 13.77 |
| ATOM | 1595 | CA  | GLY | 278 | 68.637 | 84.413 | 75.809 | 1.00 | 11.38 |
| ATOM | 1596 | C   | GLY | 278 | 68.472 | 84.918 | 74.396 | 1.00 | 11.86 |
| ATOM | 1597 | O   | GLY | 278 | 69.294 | 85.703 | 73.956 | 1.00 | 14.42 |
| ATOM | 1598 | N   | ASN | 279 | 67.460 | 84.474 | 73.664 | 1.00 | 11.99 |
| ATOM | 1599 | CA  | ASN | 279 | 67.282 | 84.959 | 72.299 | 1.00 | 13.64 |
| ATOM | 1600 | CB  | ASN | 279 | 66.599 | 83.900 | 71.438 | 1.00 | 13.49 |
| ATOM | 1601 | CG  | ASN | 279 | 66.410 | 84.345 | 70.001 | 1.00 | 12.47 |
| ATOM | 1602 | OD1 | ASN | 279 | 67.116 | 85.214 | 69.509 | 1.00 | 12.30 |
| ATOM | 1603 | ND2 | ASN | 279 | 65.435 | 83.757 | 69.331 | 1.00 | 14.37 |
| ATOM | 1604 | C   | ASN | 279 | 66.452 | 86.240 | 72.335 | 1.00 | 15.97 |
| ATOM | 1605 | O   | ASN | 279 | 65.286 | 86.256 | 71.941 | 1.00 | 18.11 |
| ATOM | 1606 | N   | SER | 280 | 67.058 | 87.317 | 72.819 | 1.00 | 16.92 |
| ATOM | 1607 | CA  | SER | 280 | 66.355 | 88.585 | 72.940 | 1.00 | 14.96 |
| ATOM | 1608 | CB  | SER | 280 | 66.005 | 88.845 | 74.408 | 1.00 | 14.71 |
| ATOM | 1609 | OG  | SER | 280 | 67.161 | 89.029 | 75.220 | 1.00 | 13.79 |
| ATOM | 1610 | C   | SER | 280 | 67.165 | 89.747 | 72.419 | 1.00 | 15.56 |
| ATOM | 1611 | O   | SER | 280 | 68.396 | 89.694 | 72.378 | 1.00 | 17.53 |
| ATOM | 1612 | N   | ILE | 281 | 66.474 | 90.825 | 72.077 | 1.00 | 15.66 |
| ATOM | 1613 | CA  | ILE | 281 | 67.135 | 92.022 | 71.584 | 1.00 | 14.41 |
| ATOM | 1614 | CB  | ILE | 281 | 66.097 | 93.080 | 71.109 | 1.00 | 14.31 |
| ATOM | 1615 | CG2 | ILE | 281 | 65.235 | 93.547 | 72.266 | 1.00 | 11.29 |
| ATOM | 1616 | CG1 | ILE | 281 | 66.807 | 94.239 | 70.417 | 1.00 | 14.68 |
| ATOM | 1617 | CD1 | ILE | 281 | 67.730 | 93.792 | 69.281 | 1.00 | 14.99 |
| ATOM | 1618 | C   | ILE | 281 | 68.042 | 92.588 | 72.683 | 1.00 | 13.74 |
| ATOM | 1619 | O   | ILE | 281 | 69.099 | 93.153 | 72.404 | 1.00 | 12.52 |
| ATOM | 1620 | N   | PHE | 282 | 67.659 | 92.368 | 73.937 | 1.00 | 15.03 |
| ATCM | 1621 | CA  | PHE | 282 | 68.435 | 92.855 | 75.077 | 1.00 | 14.86 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1622 | CB  | PHE | 282 | 67.707 | 92.591 | 76.399 | 1.00 | 14.56 |
| ATOM | 1623 | CG  | PHE | 282 | 66.256 | 92.942 | 76.364 | 1.00 | 19.88 |
| ATOM | 1624 | CD1 | PHE | 282 | 65.835 | 94.187 | 75.904 | 1.00 | 25.20 |
| ATOM | 1625 | CD2 | PHE | 282 | 65.304 | 92.026 | 76.787 | 1.00 | 22.64 |
| ATOM | 1626 | CE1 | PHE | 282 | 64.485 | 94.509 | 75.845 | 1.00 | 27.06 |
| ATOM | 1627 | CE2 | PHE | 282 | 63.951 | 92.332 | 76.735 | 1.00 | 26.16 |
| ATOM | 1628 | CZ  | PHE | 282 | 63.540 | 93.579 | 76.269 | 1.00 | 29.37 |
| ATOM | 1629 | C   | PHE | 282 | 69.796 | 92.188 | 75.122 | 1.00 | 14.34 |
| ATOM | 1630 | O   | PHE | 282 | 70.811 | 92.866 | 75.263 | 1.00 | 14.62 |
| ATOM | 1631 | N   | GLN | 283 | 69.820 | 90.864 | 75.001 | 1.00 | 15.01 |
| ATOM | 1632 | CA  | GLN | 283 | 71.087 | 90.148 | 75.052 | 1.00 | 17.13 |
| ATOM | 1633 | CB  | GLN | 283 | 70.889 | 88.660 | 75.311 | 1.00 | 17.99 |
| ATOM | 1634 | CG  | GLN | 283 | 72.196 | 87.972 | 75.692 | 1.00 | 18.78 |
| ATOM | 1635 | CD  | GLN | 283 | 72.051 | 86.486 | 75.904 | 1.00 | 16.42 |
| ATOM | 1636 | OE1 | GLN | 283 | 72.606 | 85.697 | 75.154 | 1.00 | 16.50 |
| ATOM | 1637 | NE2 | GLN | 283 | 71.322 | 86.098 | 76.944 | 1.00 | 17.31 |
| ATOM | 1638 | C   | GLN | 283 | 71.915 | 90.331 | 73.792 | 1.00 | 17.41 |
| ATOM | 1639 | O   | GLN | 283 | 73.138 | 90.426 | 73.856 | 1.00 | 17.81 |
| ATOM | 1640 | N   | ILE | 284 | 71.249 | 90.358 | 72.647 | 1.00 | 18.52 |
| ATOM | 1641 | CA  | ILE | 284 | 71.935 | 90.546 | 71.373 | 1.00 | 19.90 |
| ATOM | 1642 | CB  | ILE | 284 | 70.915 | 90.586 | 70.194 | 1.00 | 19.91 |
| ATOM | 1643 | CG2 | ILE | 284 | 71.604 | 91.001 | 68.900 | 1.00 | 20.36 |
| ATOM | 1644 | CG1 | ILE | 284 | 70.239 | 89.215 | 70.052 | 1.00 | 18.80 |
| ATOM | 1645 | CD1 | ILE | 284 | 69.221 | 89.133 | 68.948 | 1.00 | 20.66 |
| ATOM | 1646 | C   | ILE | 284 | 72.749 | 91.841 | 71.426 | 1.00 | 19.77 |
| ATOM | 1647 | O   | ILE | 284 | 73.962 | 91.831 | 71.201 | 1.00 | 21.96 |
| ATOM | 1648 | N   | ASN | 285 | 72.097 | 92.934 | 71.811 | 1.00 | 18.02 |
| ATOM | 1649 | CA  | ASN | 285 | 72.767 | 94.219 | 71.901 | 1.00 | 16.86 |
| ATOM | 1650 | CB  | ASN | 285 | 71.758 | 95.335 | 72.136 | 1.00 | 9.23  |
| ATOM | 1651 | CG  | ASN | 285 | 70.839 | 95.538 | 70.963 | 1.00 | 10.63 |
| ATOM | 1652 | OD1 | ASN | 285 | 71.251 | 95.416 | 69.805 | 1.00 | 14.11 |
| ATOM | 1653 | ND2 | ASN | 285 | 69.577 | 95.842 | 71.246 | 1.00 | 12.07 |
| ATOM | 1654 | C   | ASN | 285 | 73.842 | 94.223 | 72.980 | 1.00 | 19.52 |
| ATOM | 1655 | O   | ASN | 285 | 74.877 | 94.881 | 72.838 | 1.00 | 21.75 |
| ATOM | 1656 | N   | MET | 286 | 73.610 | 93.474 | 74.051 | 1.00 | 20.87 |
| ATOM | 1657 | CA  | MET | 286 | 74.582 | 93.388 | 75.132 | 1.00 | 24.40 |
| ATOM | 1658 | CB  | MET | 286 | 73.979 | 92.662 | 76.335 | 1.00 | 25.20 |
| ATOM | 1659 | CG  | MET | 286 | 74.934 | 92.449 | 77.501 | 1.00 | 29.91 |
| ATOM | 1660 | SD  | MET | 286 | 75.778 | 93.921 | 78.086 | 1.00 | 26.75 |
| ATOM | 1661 | CE  | MET | 286 | 74.626 | 94.506 | 79.322 | 1.00 | 30.56 |
| ATOM | 1662 | C   | MET | 286 | 75.831 | 92.666 | 74.621 | 1.00 | 27.07 |
| ATOM | 1663 | O   | MET | 286 | 76.958 | 93.069 | 74.930 | 1.00 | 27.63 |
| ATOM | 1664 | N   | ILE | 287 | 75.621 | 91.634 | 73.803 | 1.00 | 28.55 |
| ATOM | 1665 | CA  | ILE | 287 | 76.712 | 90.856 | 73.215 | 1.00 | 28.03 |
| ATOM | 1666 | CB  | ILE | 287 | 76.175 | 89.730 | 72.294 | 1.00 | 26.14 |
| ATOM | 1667 | CG2 | ILE | 287 | 77.310 | 89.112 | 71.487 | 1.00 | 23.50 |
| ATOM | 1668 | CG1 | ILE | 287 | 75.472 | 88.648 | 73.114 | 1.00 | 26.20 |
| ATOM | 1669 | CD1 | ILE | 287 | 76.414 | 87.729 | 73.835 | 1.00 | 24.06 |
| ATOM | 1670 | C   | ILE | 287 | 77.556 | 91.794 | 72.362 | 1.00 | 29.78 |
| ATOM | 1671 | O   | ILE | 287 | 78.770 | 91.906 | 72.559 | 1.00 | 30.63 |
| ATOM | 1672 | N   | LYS | 288 | 76.892 | 92.483 | 71.437 | 1.00 | 31.89 |
| ATOM | 1673 | CA  | LYS | 288 | 77.549 | 93.417 | 70.523 | 1.00 | 34.53 |
| ATOM | 1674 | CB  | LYS | 288 | 76.521 | 94.076 | 69.603 | 1.00 | 33.65 |
| ATOM | 1675 | CG  | LYS | 288 | 75.860 | 93.124 | 68.623 | 1.00 | 33.76 |
| ATOM | 1676 | CD  | LYS | 288 | 74.914 | 93.876 | 67.713 | 1.00 | 38.36 |
| ATOM | 1677 | CE  | LYS | 288 | 74.279 | 92.962 | 66.684 | 1.00 | 43.07 |
| ATOM | 1678 | NZ  | LYS | 288 | 73.338 | 93.710 | 65.798 | 1.00 | 47.95 |
| ATOM | 1679 | C   | LYS | 288 | 78.343 | 94.485 | 71.265 | 1.00 | 37.00 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |         |        |      |       |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 1680 | O   | LYS | 288 | 79.420 | 94.897  | 70.819 | 1.00 | 39.41 |
| ATOM | 1681 | N   | TYR | 289 | 77.790 | 94.945  | 72.383 | 1.00 | 36.27 |
| ATOM | 1682 | CA  | TYR | 289 | 78.436 | 95.944  | 73.219 | 1.00 | 34.85 |
| ATOM | 1683 | CB  | TYR | 289 | 77.514 | 96.292  | 74.390 | 1.00 | 32.73 |
| ATOM | 1684 | CG  | TYR | 289 | 78.159 | 97.114  | 75.482 | 1.00 | 30.62 |
| ATOM | 1685 | CD1 | TYR | 289 | 78.359 | 98.484  | 75.327 | 1.00 | 31.85 |
| ATOM | 1686 | CE1 | TYR | 289 | 78.943 | 99.243  | 76.325 | 1.00 | 28.71 |
| ATOM | 1687 | CD2 | TYR | 289 | 78.574 | 96.522  | 76.668 | 1.00 | 31.04 |
| ATOM | 1688 | CE2 | TYR | 289 | 79.162 | 97.273  | 77.675 | 1.00 | 31.98 |
| ATOM | 1689 | CZ  | TYR | 289 | 79.348 | 98.630  | 77.494 | 1.00 | 30.03 |
| ATOM | 1690 | OH  | TYR | 289 | 79.931 | 99.374  | 78.485 | 1.00 | 32.92 |
| ATOM | 1691 | C   | TYR | 289 | 79.770 | 95.401  | 73.744 | 1.00 | 35.05 |
| ATOM | 1692 | O   | TYR | 289 | 80.833 | 95.979  | 73.507 | 1.00 | 34.75 |
| ATOM | 1693 | N   | MET | 290 | 79.697 | 94.261  | 74.421 | 1.00 | 35.07 |
| ATOM | 1694 | CA  | MET | 290 | 80.858 | 93.611  | 75.011 | 1.00 | 34.69 |
| ATOM | 1695 | CB  | MET | 290 | 80.422 | 92.339  | 75.727 | 1.00 | 33.03 |
| ATOM | 1696 | CG  | MET | 290 | 79.436 | 92.601  | 76.840 | 1.00 | 31.76 |
| ATOM | 1697 | SD  | MET | 290 | 78.883 | 91.099  | 77.601 | 1.00 | 31.65 |
| ATOM | 1698 | CE  | MET | 290 | 80.424 | 90.507  | 78.341 | 1.00 | 30.46 |
| ATOM | 1699 | C   | MET | 290 | 81.958 | 93.295  | 74.012 | 1.00 | 36.51 |
| ATOM | 1700 | O   | MET | 290 | 83.141 | 93.486  | 74.308 | 1.00 | 37.23 |
| ATOM | 1701 | N   | LYS | 291 | 81.577 | 92.788  | 72.843 | 1.00 | 36.05 |
| ATOM | 1702 | CA  | LYS | 291 | 82.550 | 92.458  | 71.803 | 1.00 | 34.69 |
| ATOM | 1703 | CB  | LYS | 291 | 81.856 | 91.770  | 70.626 | 1.00 | 35.82 |
| ATOM | 1704 | CG  | LYS | 291 | 82.396 | 90.391  | 70.284 | 1.00 | 36.35 |
| ATOM | 1705 | CD  | LYS | 291 | 82.164 | 89.404  | 71.417 | 1.00 | 38.70 |
| ATOM | 1706 | CE  | LYS | 291 | 83.442 | 89.107  | 72.198 | 1.00 | 38.01 |
| ATOM | 1707 | NZ  | LYS | 291 | 84.404 | 88.262  | 71.437 | 1.00 | 33.80 |
| ATOM | 1708 | C   | LYS | 291 | 83.243 | 93.733  | 71.328 | 1.00 | 34.40 |
| ATOM | 1709 | O   | LYS | 291 | 84.393 | 93.699  | 70.897 | 1.00 | 33.76 |
| ATOM | 1710 | N   | GLU | 292 | 82.528 | 94.853  | 71.401 | 1.00 | 34.73 |
| ATOM | 1711 | CA  | GLU | 292 | 83.063 | 96.145  | 70.998 | 1.00 | 35.38 |
| ATOM | 1712 | CB  | GLU | 292 | 81.933 | 97.156  | 70.798 | 1.00 | 41.72 |
| ATOM | 1713 | CG  | GLU | 292 | 82.425 | 98.589  | 70.606 | 1.00 | 53.68 |
| ATOM | 1714 | CD  | GLU | 292 | 81.320 | 99.627  | 70.724 | 1.00 | 64.47 |
| ATOM | 1715 | OE1 | GLU | 292 | 81.251 | 100.519 | 69.847 | 1.00 | 68.28 |
| ATOM | 1716 | OE2 | GLU | 292 | 80.533 | 99.564  | 71.698 | 1.00 | 69.72 |
| ATOM | 1717 | C   | GLU | 292 | 84.021 | 96.681  | 72.051 | 1.00 | 33.49 |
| ATOM | 1718 | O   | GLU | 292 | 85.194 | 96.928  | 71.773 | 1.00 | 32.22 |
| ATOM | 1719 | N   | LYS | 293 | 83.503 | 96.868  | 73.259 | 1.00 | 32.85 |
| ATOM | 1720 | CA  | LYS | 293 | 84.286 | 97.395  | 74.372 | 1.00 | 32.45 |
| ATOM | 1721 | CB  | LYS | 293 | 83.386 | 97.603  | 75.592 | 1.00 | 30.22 |
| ATOM | 1722 | CG  | LYS | 293 | 83.986 | 98.489  | 76.659 | 1.00 | 29.87 |
| ATOM | 1723 | CD  | LYS | 293 | 83.036 | 98.648  | 77.822 | 1.00 | 32.75 |
| ATOM | 1724 | CE  | LYS | 293 | 83.579 | 99.596  | 78.874 | 1.00 | 34.50 |
| ATOM | 1725 | NZ  | LYS | 293 | 83.695 | 100.990 | 78.367 | 1.00 | 40.11 |
| ATOM | 1726 | C   | LYS | 293 | 85.458 | 96.493  | 74.745 | 1.00 | 32.68 |
| ATOM | 1727 | O   | LYS | 293 | 86.563 | 96.971  | 74.990 | 1.00 | 33.81 |
| ATOM | 1728 | N   | TYR | 294 | 85.212 | 95.190  | 74.781 | 1.00 | 32.79 |
| ATOM | 1729 | CA  | TYR | 294 | 86.233 | 94.216  | 75.135 | 1.00 | 33.40 |
| ATOM | 1730 | CB  | TYR | 294 | 85.822 | 93.506  | 76.428 | 1.00 | 30.64 |
| ATOM | 1731 | CG  | TYR | 294 | 85.685 | 94.421  | 77.628 | 1.00 | 27.56 |
| ATOM | 1732 | CD1 | TYR | 294 | 86.817 | 94.950  | 78.251 | 1.00 | 27.07 |
| ATOM | 1733 | CE1 | TYR | 294 | 86.713 | 95.786  | 79.358 | 1.00 | 25.34 |
| ATOM | 1734 | CD2 | TYR | 294 | 84.432 | 94.754  | 78.146 | 1.00 | 26.35 |
| ATOM | 1735 | CE2 | TYR | 294 | 84.314 | 95.591  | 79.259 | 1.00 | 25.10 |
| ATOM | 1736 | CZ  | TYR | 294 | 85.463 | 96.102  | 79.856 | 1.00 | 27.67 |
| ATOM | 1737 | OH  | TYR | 294 | 85.378 | 96.923  | 80.955 | 1.00 | 29.72 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1738 | C   | TYR | 294 | 86.385 | 93.202 | 74.005 | 1.00 | 35.70 |
| ATOM | 1739 | O   | TYR | 294 | 86.004 | 92.048 | 74.153 | 1.00 | 36.93 |
| ATOM | 1740 | N   | PRO | 295 | 87.047 | 93.594 | 72.904 | 1.00 | 37.78 |
| ATOM | 1741 | CD  | PRO | 295 | 87.797 | 94.854 | 72.787 | 1.00 | 38.64 |
| ATOM | 1742 | CA  | PRO | 295 | 87.276 | 92.755 | 71.720 | 1.00 | 38.05 |
| ATOM | 1743 | CB  | PRO | 295 | 88.340 | 93.532 | 70.952 | 1.00 | 38.38 |
| ATOM | 1744 | CG  | PRO | 295 | 88.039 | 94.939 | 71.301 | 1.00 | 41.28 |
| ATOM | 1745 | C   | PRO | 295 | 87.749 | 91.334 | 71.982 | 1.00 | 39.01 |
| ATOM | 1746 | O   | PRO | 295 | 87.333 | 90.401 | 71.295 | 1.00 | 41.67 |
| ATOM | 1747 | N   | ASN | 296 | 88.625 | 91.172 | 72.965 | 1.00 | 37.89 |
| ATOM | 1748 | CA  | ASN | 296 | 89.174 | 89.859 | 73.274 | 1.00 | 38.39 |
| ATOM | 1749 | CB  | ASN | 296 | 90.623 | 89.999 | 73.747 | 1.00 | 45.75 |
| ATOM | 1750 | CG  | ASN | 296 | 91.562 | 90.469 | 72.645 | 1.00 | 53.22 |
| ATOM | 1751 | OD1 | ASN | 296 | 91.127 | 91.015 | 71.627 | 1.00 | 58.39 |
| ATOM | 1752 | ND2 | ASN | 296 | 92.860 | 90.266 | 72.850 | 1.00 | 54.67 |
| ATOM | 1753 | C   | ASN | 296 | 88.393 | 89.020 | 74.280 | 1.00 | 37.03 |
| ATOM | 1754 | O   | ASN | 296 | 88.561 | 87.796 | 74.329 | 1.00 | 39.51 |
| ATOM | 1755 | N   | LEU | 297 | 87.531 | 89.664 | 75.066 | 1.00 | 33.27 |
| ATOM | 1756 | CA  | LEU | 297 | 86.754 | 88.965 | 76.086 | 1.00 | 27.99 |
| ATOM | 1757 | CB  | LEU | 297 | 85.902 | 89.945 | 76.898 | 1.00 | 23.39 |
| ATOM | 1758 | CG  | LEU | 297 | 85.183 | 89.404 | 78.137 | 1.00 | 19.80 |
| ATOM | 1759 | CD1 | LEU | 297 | 86.188 | 88.783 | 79.104 | 1.00 | 12.69 |
| ATOM | 1760 | CD2 | LEU | 297 | 84.389 | 90.524 | 78.805 | 1.00 | 14.38 |
| ATOM | 1761 | C   | LEU | 297 | 85.872 | 87.884 | 75.492 | 1.00 | 27.28 |
| ATOM | 1762 | O   | LEU | 297 | 85.189 | 88.096 | 74.491 | 1.00 | 28.13 |
| ATOM | 1763 | N   | GLN | 298 | 85.906 | 86.715 | 76.116 | 1.00 | 26.76 |
| ATOM | 1764 | CA  | GLN | 298 | 85.122 | 85.577 | 75.670 | 1.00 | 23.04 |
| ATOM | 1765 | CB  | GLN | 298 | 85.814 | 84.292 | 76.090 | 1.00 | 22.03 |
| ATOM | 1766 | CG  | GLN | 298 | 87.125 | 84.068 | 75.373 | 1.00 | 20.61 |
| ATOM | 1767 | CD  | GLN | 298 | 86.930 | 83.836 | 73.887 | 1.00 | 23.42 |
| ATOM | 1768 | OE1 | GLN | 298 | 86.604 | 82.728 | 73.459 | 1.00 | 22.37 |
| ATOM | 1769 | NE2 | GLN | 298 | 87.125 | 84.877 | 73.092 | 1.00 | 23.24 |
| ATOM | 1770 | C   | GLN | 298 | 83.719 | 85.643 | 76.249 | 1.00 | 22.42 |
| ATOM | 1771 | O   | GLN | 298 | 83.544 | 85.639 | 77.468 | 1.00 | 22.91 |
| ATOM | 1772 | N   | VAL | 299 | 82.728 | 85.712 | 75.365 | 1.00 | 20.33 |
| ATOM | 1773 | CA  | VAL | 299 | 81.333 | 85.797 | 75.767 | 1.00 | 17.94 |
| ATOM | 1774 | CB  | VAL | 299 | 80.690 | 87.048 | 75.161 | 1.00 | 18.36 |
| ATOM | 1775 | CG1 | VAL | 299 | 79.317 | 87.271 | 75.737 | 1.00 | 16.17 |
| ATOM | 1776 | CG2 | VAL | 299 | 81.578 | 88.257 | 75.410 | 1.00 | 20.86 |
| ATOM | 1777 | C   | VAL | 299 | 80.523 | 84.549 | 75.379 | 1.00 | 17.77 |
| ATOM | 1778 | O   | VAL | 299 | 80.683 | 83.997 | 74.287 | 1.00 | 17.61 |
| ATOM | 1779 | N   | ILE | 300 | 79.655 | 84.121 | 76.291 | 1.00 | 15.64 |
| ATOM | 1780 | CA  | ILE | 300 | 78.803 | 82.955 | 76.113 | 1.00 | 11.70 |
| ATOM | 1781 | CB  | ILE | 300 | 79.026 | 81.983 | 77.276 | 1.00 | 5.27  |
| ATOM | 1782 | CG2 | ILE | 300 | 78.130 | 80.794 | 77.157 | 1.00 | 9.90  |
| ATOM | 1783 | CG1 | ILE | 300 | 80.485 | 81.544 | 77.289 | 1.00 | 3.10  |
| ATOM | 1784 | CD1 | ILE | 300 | 80.845 | 80.697 | 78.471 | 1.00 | 6.58  |
| ATOM | 1785 | C   | ILE | 300 | 77.340 | 83.423 | 76.059 | 1.00 | 13.85 |
| ATOM | 1786 | O   | ILE | 300 | 76.928 | 84.238 | 76.876 | 1.00 | 13.73 |
| ATOM | 1787 | N   | GLY | 301 | 76.569 | 82.902 | 75.105 | 1.00 | 16.05 |
| ATOM | 1788 | CA  | GLY | 301 | 75.184 | 83.312 | 74.929 | 1.00 | 18.06 |
| ATOM | 1789 | C   | GLY | 301 | 74.134 | 82.665 | 75.804 | 1.00 | 20.81 |
| ATOM | 1790 | O   | GLY | 301 | 74.131 | 81.445 | 75.958 | 1.00 | 21.22 |
| ATOM | 1791 | N   | GLY | 302 | 73.240 | 83.512 | 76.330 | 1.00 | 23.53 |
| ATOM | 1792 | CA  | GLY | 302 | 72.133 | 83.145 | 77.218 | 1.00 | 22.62 |
| ATOM | 1793 | C   | GLY | 302 | 71.470 | 81.838 | 76.874 | 1.00 | 23.12 |
| ATOM | 1794 | O   | GLY | 302 | 71.613 | 81.391 | 75.733 | 1.00 | 26.43 |
| ATOM | 1795 | N   | ASN | 303 | 70.684 | 81.263 | 77.791 | 1.00 | 18.57 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1796 | CA  | ASN | 303 | 70.089 | 79.951 | 77.516 | 1.00 | 14.15 |
| ATOM | 1797 | CB  | ASN | 303 | 69.434 | 79.345 | 78.750 | 1.00 | 10.27 |
| ATOM | 1798 | CG  | ASN | 303 | 70.445 | 78.700 | 79.679 | 1.00 | 13.65 |
| ATOM | 1799 | OD1 | ASN | 303 | 70.297 | 77.553 | 80.098 | 1.00 | 14.49 |
| ATOM | 1800 | ND2 | ASN | 303 | 71.503 | 79.438 | 79.989 | 1.00 | 12.02 |
| ATOM | 1801 | C   | ASN | 303 | 69.212 | 79.796 | 76.301 | 1.00 | 12.10 |
| ATOM | 1802 | O   | ASN | 303 | 68.194 | 80.475 | 76.161 | 1.00 | 13.68 |
| ATOM | 1803 | N   | VAL | 304 | 69.668 | 78.936 | 75.390 | 1.00 | 9.70  |
| ATOM | 1804 | CA  | VAL | 304 | 68.963 | 78.635 | 74.149 | 1.00 | 9.71  |
| ATOM | 1805 | CB  | VAL | 304 | 69.712 | 79.185 | 72.881 | 1.00 | 9.64  |
| ATOM | 1806 | CG1 | VAL | 304 | 69.948 | 80.697 | 72.987 | 1.00 | 5.85  |
| ATOM | 1807 | CG2 | VAL | 304 | 71.030 | 78.454 | 72.654 | 1.00 | 4.29  |
| ATOM | 1808 | C   | VAL | 304 | 68.774 | 77.123 | 73.999 | 1.00 | 10.42 |
| ATOM | 1809 | O   | VAL | 304 | 69.493 | 76.325 | 74.619 | 1.00 | 8.79  |
| ATOM | 1810 | N   | VAL | 305 | 67.785 | 76.731 | 73.200 | 1.00 | 10.37 |
| ATOM | 1811 | CA  | VAL | 305 | 67.510 | 75.313 | 72.963 | 1.00 | 9.42  |
| ATOM | 1812 | CB  | VAL | 305 | 66.380 | 74.769 | 73.899 | 1.00 | 9.04  |
| ATOM | 1813 | CG1 | VAL | 305 | 66.785 | 74.892 | 75.349 | 1.00 | 6.04  |
| ATOM | 1814 | CG2 | VAL | 305 | 65.069 | 75.492 | 73.652 | 1.00 | 9.90  |
| ATOM | 1815 | C   | VAL | 305 | 67.187 | 74.978 | 71.498 | 1.00 | 9.35  |
| ATOM | 1816 | O   | VAL | 305 | 66.936 | 73.823 | 71.172 | 1.00 | 9.44  |
| ATOM | 1817 | N   | THR | 306 | 67.212 | 75.977 | 70.617 | 1.00 | 9.59  |
| ATOM | 1818 | CA  | THR | 306 | 66.929 | 75.762 | 69.197 | 1.00 | 11.26 |
| ATOM | 1819 | CB  | THR | 306 | 65.522 | 76.277 | 68.796 | 1.00 | 15.29 |
| ATOM | 1820 | OG1 | THR | 306 | 65.485 | 77.702 | 68.918 | 1.00 | 24.72 |
| ATOM | 1821 | CG2 | THR | 306 | 64.427 | 75.679 | 69.673 | 1.00 | 13.39 |
| ATOM | 1822 | C   | THR | 306 | 67.960 | 76.493 | 68.331 | 1.00 | 12.58 |
| ATOM | 1823 | O   | THR | 306 | 68.531 | 77.502 | 68.748 | 1.00 | 11.97 |
| ATOM | 1824 | N   | ALA | 307 | 68.164 | 76.001 | 67.112 | 1.00 | 13.41 |
| ATOM | 1825 | CA  | ALA | 307 | 69.118 | 76.593 | 66.181 | 1.00 | 12.33 |
| ATOM | 1826 | CB  | ALA | 307 | 69.226 | 75.725 | 64.947 | 1.00 | 10.43 |
| ATOM | 1827 | C   | ALA | 307 | 68.764 | 78.035 | 65.794 | 1.00 | 14.20 |
| ATOM | 1828 | O   | ALA | 307 | 69.645 | 78.870 | 65.605 | 1.00 | 17.80 |
| ATOM | 1829 | N   | ALA | 308 | 67.477 | 78.328 | 65.670 | 1.00 | 14.93 |
| ATOM | 1830 | CA  | ALA | 308 | 67.031 | 79.671 | 65.324 | 1.00 | 14.54 |
| ATOM | 1831 | CB  | ALA | 308 | 65.529 | 79.700 | 65.176 | 1.00 | 11.96 |
| ATOM | 1832 | C   | ALA | 308 | 67.488 | 80.675 | 66.390 | 1.00 | 17.15 |
| ATOM | 1833 | O   | ALA | 308 | 67.893 | 81.790 | 66.060 | 1.00 | 18.96 |
| ATOM | 1834 | N   | GLN | 309 | 67.412 | 80.281 | 67.663 | 1.00 | 17.15 |
| ATOM | 1835 | CA  | GLN | 309 | 67.844 | 81.146 | 68.762 | 1.00 | 17.48 |
| ATOM | 1836 | CB  | GLN | 309 | 67.486 | 80.545 | 70.117 | 1.00 | 15.04 |
| ATOM | 1837 | CG  | GLN | 309 | 66.015 | 80.443 | 70.439 | 1.00 | 11.07 |
| ATOM | 1838 | CD  | GLN | 309 | 65.813 | 79.776 | 71.777 | 1.00 | 11.92 |
| ATOM | 1839 | OE1 | GLN | 309 | 65.754 | 80.431 | 72.816 | 1.00 | 15.82 |
| ATOM | 1840 | NE2 | GLN | 309 | 65.783 | 78.461 | 71.769 | 1.00 | 11.54 |
| ATOM | 1841 | C   | GLN | 309 | 69.361 | 81.291 | 68.704 | 1.00 | 19.46 |
| ATOM | 1842 | O   | GLN | 309 | 69.899 | 82.400 | 68.800 | 1.00 | 22.14 |
| ATOM | 1843 | N   | ALA | 310 | 70.048 | 80.162 | 68.577 | 1.00 | 18.81 |
| ATOM | 1844 | CA  | ALA | 310 | 71.502 | 80.158 | 68.510 | 1.00 | 19.07 |
| ATOM | 1845 | CB  | ALA | 310 | 72.027 | 78.744 | 68.259 | 1.00 | 16.86 |
| ATOM | 1846 | C   | ALA | 310 | 71.997 | 81.107 | 67.429 | 1.00 | 20.18 |
| ATOM | 1847 | O   | ALA | 310 | 72.896 | 81.907 | 67.685 | 1.00 | 21.07 |
| ATOM | 1848 | N   | LYS | 311 | 71.368 | 81.071 | 66.253 | 1.00 | 19.18 |
| ATOM | 1849 | CA  | LYS | 311 | 71.776 | 81.935 | 65.150 | 1.00 | 18.89 |
| ATOM | 1850 | CB  | LYS | 311 | 70.870 | 81.777 | 63.934 | 1.00 | 19.89 |
| ATOM | 1851 | CG  | LYS | 311 | 71.413 | 82.571 | 62.752 | 1.00 | 22.42 |
| ATOM | 1852 | CD  | LYS | 311 | 70.399 | 82.826 | 61.664 | 1.00 | 23.48 |
| ATOM | 1853 | CE  | LYS | 311 | 71.067 | 83.538 | 60.499 | 1.00 | 26.29 |



FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1854 | NZ  | LYS | 311 | 72.227 | 82.755 | 59.948 | 1.00 | 28.08 |
| ATOM | 1855 | C   | LYS | 311 | 71.838 | 83.414 | 65.508 | 1.00 | 18.94 |
| ATOM | 1856 | O   | LYS | 311 | 72.763 | 84.113 | 65.096 | 1.00 | 20.88 |
| ATOM | 1857 | N   | ASN | 312 | 70.843 | 83.912 | 66.235 | 1.00 | 17.97 |
| ATOM | 1858 | CA  | ASN | 312 | 70.849 | 85.319 | 66.611 | 1.00 | 19.27 |
| ATOM | 1859 | CB  | ASN | 312 | 69.543 | 85.713 | 67.295 | 1.00 | 21.83 |
| ATOM | 1860 | CG  | ASN | 312 | 68.409 | 85.916 | 66.311 | 1.00 | 28.87 |
| ATOM | 1861 | OD1 | ASN | 312 | 67.238 | 85.717 | 66.642 | 1.00 | 31.90 |
| ATOM | 1862 | ND2 | ASN | 312 | 68.747 | 86.338 | 65.094 | 1.00 | 29.09 |
| ATOM | 1863 | C   | ASN | 312 | 72.037 | 85.665 | 67.497 | 1.00 | 20.98 |
| ATOM | 1864 | O   | ASN | 312 | 72.734 | 86.661 | 67.258 | 1.00 | 22.46 |
| ATOM | 1865 | N   | LEU | 313 | 72.292 | 84.821 | 68.494 | 1.00 | 21.52 |
| ATOM | 1866 | CA  | LEU | 313 | 73.399 | 85.032 | 69.420 | 1.00 | 20.77 |
| ATOM | 1867 | CB  | LEU | 313 | 73.259 | 84.117 | 70.639 | 1.00 | 17.46 |
| ATOM | 1868 | CG  | LEU | 313 | 71.923 | 84.136 | 71.385 | 1.00 | 6.88  |
| ATOM | 1869 | CD1 | LEU | 313 | 72.126 | 83.569 | 72.760 | 1.00 | 9.49  |
| ATOM | 1870 | CD2 | LEU | 313 | 71.395 | 85.532 | 71.497 | 1.00 | 3.00  |
| ATOM | 1871 | C   | LEU | 313 | 74.745 | 84.807 | 68.723 | 1.00 | 22.50 |
| ATOM | 1872 | O   | LEU | 313 | 75.739 | 85.481 | 69.022 | 1.00 | 24.58 |
| ATOM | 1873 | N   | ILE | 314 | 74.781 | 83.856 | 67.798 | 1.00 | 21.23 |
| ATOM | 1874 | CA  | ILE | 314 | 75.993 | 83.579 | 67.049 | 1.00 | 20.90 |
| ATOM | 1875 | CB  | ILE | 314 | 75.846 | 82.316 | 66.175 | 1.00 | 21.15 |
| ATOM | 1876 | CG2 | ILE | 314 | 76.962 | 82.257 | 65.143 | 1.00 | 23.20 |
| ATOM | 1877 | CG1 | ILE | 314 | 75.842 | 81.062 | 67.062 | 1.00 | 20.42 |
| ATOM | 1878 | CD1 | ILE | 314 | 75.839 | 79.736 | 66.299 | 1.00 | 14.79 |
| ATOM | 1879 | C   | ILE | 314 | 76.281 | 84.806 | 66.181 | 1.00 | 22.74 |
| ATOM | 1880 | O   | ILE | 314 | 77.417 | 85.285 | 66.129 | 1.00 | 23.40 |
| ATOM | 1881 | N   | ASP | 315 | 75.241 | 85.338 | 65.540 | 1.00 | 22.48 |
| ATOM | 1882 | CA  | ASP | 315 | 75.378 | 86.528 | 64.700 | 1.00 | 22.51 |
| ATOM | 1883 | CB  | ASP | 315 | 74.060 | 86.854 | 63.997 | 1.00 | 21.37 |
| ATOM | 1884 | CG  | ASP | 315 | 73.766 | 85.937 | 62.828 | 1.00 | 20.01 |
| ATOM | 1885 | OD1 | ASP | 315 | 74.687 | 85.252 | 62.339 | 1.00 | 20.88 |
| ATOM | 1886 | OD2 | ASP | 315 | 72.605 | 85.925 | 62.377 | 1.00 | 17.86 |
| ATOM | 1887 | C   | ASP | 315 | 75.790 | 87.723 | 65.555 | 1.00 | 23.82 |
| ATOM | 1888 | O   | ASP | 315 | 76.536 | 88.585 | 65.104 | 1.00 | 24.06 |
| ATOM | 1889 | N   | ALA | 316 | 75.270 | 87.787 | 66.779 | 1.00 | 23.31 |
| ATOM | 1890 | CA  | ALA | 316 | 75.602 | 88.868 | 67.691 | 1.00 | 21.76 |
| ATOM | 1891 | CB  | ALA | 316 | 74.737 | 88.798 | 68.928 | 1.00 | 23.15 |
| ATOM | 1892 | C   | ALA | 316 | 77.074 | 88.770 | 68.063 | 1.00 | 22.92 |
| ATOM | 1893 | O   | ALA | 316 | 77.651 | 89.726 | 68.558 | 1.00 | 24.54 |
| ATOM | 1894 | N   | GLY | 317 | 77.658 | 87.587 | 67.881 | 1.00 | 24.30 |
| ATOM | 1895 | CA  | GLY | 317 | 79.073 | 87.395 | 68.160 | 1.00 | 24.83 |
| ATOM | 1896 | C   | GLY | 317 | 79.476 | 86.539 | 69.350 | 1.00 | 24.46 |
| ATOM | 1897 | O   | GLY | 317 | 80.532 | 86.763 | 69.931 | 1.00 | 25.80 |
| ATOM | 1898 | N   | VAL | 318 | 78.672 | 85.545 | 69.710 | 1.00 | 22.39 |
| ATOM | 1899 | CA  | VAL | 318 | 79.015 | 84.702 | 70.850 | 1.00 | 18.88 |
| ATOM | 1900 | CB  | VAL | 318 | 77.820 | 83.880 | 71.330 | 1.00 | 16.89 |
| ATOM | 1901 | CG1 | VAL | 318 | 76.731 | 84.793 | 71.846 | 1.00 | 15.19 |
| ATOM | 1902 | CG2 | VAL | 318 | 77.301 | 83.005 | 70.206 | 1.00 | 17.48 |
| ATOM | 1903 | C   | VAL | 318 | 80.185 | 83.760 | 70.586 | 1.00 | 18.75 |
| ATOM | 1904 | O   | VAL | 318 | 80.346 | 83.231 | 69.483 | 1.00 | 18.57 |
| ATOM | 1905 | N   | ASP | 319 | 80.996 | 83.551 | 71.617 | 1.00 | 17.81 |
| ATOM | 1906 | CA  | ASP | 319 | 82.148 | 82.665 | 71.529 | 1.00 | 16.90 |
| ATOM | 1907 | CB  | ASP | 319 | 83.286 | 83.188 | 72.406 | 1.00 | 20.18 |
| ATOM | 1908 | CG  | ASP | 319 | 83.865 | 84.483 | 71.895 | 1.00 | 21.11 |
| ATOM | 1909 | OD1 | ASP | 319 | 84.463 | 84.475 | 70.797 | 1.00 | 24.71 |
| ATOM | 1910 | OD2 | ASP | 319 | 83.727 | 85.508 | 72.594 | 1.00 | 21.10 |
| ATOM | 1911 | C   | ASP | 319 | 81.802 | 81.242 | 71.951 | 1.00 | 14.69 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1912 | O   | ASP | 319 | 82.640 | 80.353 | 71.870 | 1.00 | 16.26 |
| ATOM | 1913 | N   | ALA | 320 | 80.593 | 81.055 | 72.464 | 1.00 | 11.91 |
| ATOM | 1914 | CA  | ALA | 320 | 80.102 | 79.758 | 72.914 | 1.00 | 7.79  |
| ATOM | 1915 | CB  | ALA | 320 | 80.830 | 79.315 | 74.163 | 1.00 | 3.09  |
| ATOM | 1916 | C   | ALA | 320 | 78.632 | 79.953 | 73.218 | 1.00 | 8.10  |
| ATOM | 1917 | O   | ALA | 320 | 78.165 | 81.092 | 73.284 | 1.00 | 9.40  |
| ATOM | 1918 | N   | LEU | 321 | 77.900 | 78.856 | 73.404 | 1.00 | 8.90  |
| ATOM | 1919 | CA  | LEU | 321 | 76.467 | 78.917 | 73.713 | 1.00 | 6.89  |
| ATOM | 1920 | CB  | LEU | 321 | 75.645 | 78.427 | 72.529 | 1.00 | 2.00  |
| ATOM | 1921 | CG  | LEU | 321 | 75.538 | 79.283 | 71.268 | 1.00 | 2.00  |
| ATOM | 1922 | CD1 | LEU | 321 | 75.062 | 78.394 | 70.158 | 1.00 | 4.37  |
| ATOM | 1923 | CD2 | LEU | 321 | 74.589 | 80.461 | 71.444 | 1.00 | 2.00  |
| ATOM | 1924 | C   | LEU | 321 | 76.121 | 78.088 | 74.947 | 1.00 | 8.16  |
| ATOM | 1925 | O   | LEU | 321 | 76.665 | 77.008 | 75.144 | 1.00 | 10.39 |
| ATOM | 1926 | N   | ARG | 322 | 75.258 | 78.618 | 75.804 | 1.00 | 7.97  |
| ATOM | 1927 | CA  | ARG | 322 | 74.836 | 77.907 | 77.001 | 1.00 | 7.47  |
| ATOM | 1928 | CB  | ARG | 322 | 74.697 | 78.883 | 78.168 | 1.00 | 9.30  |
| ATOM | 1929 | CG  | ARG | 322 | 74.550 | 78.234 | 79.535 | 1.00 | 15.10 |
| ATOM | 1930 | CD  | ARG | 322 | 74.657 | 79.288 | 80.642 | 1.00 | 18.83 |
| ATOM | 1931 | NE  | ARG | 322 | 74.309 | 78.765 | 81.965 | 1.00 | 18.29 |
| ATOM | 1932 | CZ  | ARG | 322 | 73.750 | 79.488 | 82.932 | 1.00 | 17.03 |
| ATOM | 1933 | NH1 | ARG | 322 | 73.483 | 80.771 | 82.740 | 1.00 | 18.79 |
| ATOM | 1934 | NH2 | ARG | 322 | 73.411 | 78.921 | 84.078 | 1.00 | 16.70 |
| ATOM | 1935 | C   | ARG | 322 | 73.486 | 77.329 | 76.602 | 1.00 | 8.75  |
| ATOM | 1936 | O   | ARG | 322 | 72.535 | 78.071 | 76.373 | 1.00 | 10.16 |
| ATOM | 1937 | N   | VAL | 323 | 73.424 | 76.012 | 76.455 | 1.00 | 8.83  |
| ATOM | 1938 | CA  | VAL | 323 | 72.209 | 75.346 | 76.023 | 1.00 | 10.03 |
| ATOM | 1939 | CB  | VAL | 323 | 72.523 | 74.365 | 74.871 | 1.00 | 9.77  |
| ATOM | 1940 | CG1 | VAL | 323 | 71.306 | 73.549 | 74.507 | 1.00 | 16.85 |
| ATOM | 1941 | CG2 | VAL | 323 | 72.993 | 75.137 | 73.653 | 1.00 | 7.40  |
| ATOM | 1942 | C   | VAL | 323 | 71.473 | 74.633 | 77.153 | 1.00 | 13.18 |
| ATOM | 1943 | O   | VAL | 323 | 72.053 | 73.803 | 77.853 | 1.00 | 15.89 |
| ATOM | 1944 | N   | GLY | 324 | 70.196 | 74.969 | 77.327 | 1.00 | 12.40 |
| ATOM | 1945 | CA  | GLY | 324 | 69.392 | 74.347 | 78.362 | 1.00 | 13.80 |
| ATOM | 1946 | C   | GLY | 324 | 68.211 | 75.201 | 78.791 | 1.00 | 14.53 |
| ATOM | 1947 | O   | GLY | 324 | 68.367 | 76.397 | 78.997 | 1.00 | 17.39 |
| ATOM | 1948 | N   | MET | 325 | 67.026 | 74.613 | 78.901 | 1.00 | 11.83 |
| ATOM | 1949 | CA  | MET | 325 | 65.868 | 75.368 | 79.341 | 1.00 | 13.08 |
| ATOM | 1950 | CB  | MET | 325 | 65.201 | 76.124 | 78.186 | 1.00 | 12.41 |
| ATOM | 1951 | CG  | MET | 325 | 64.150 | 77.118 | 78.678 | 1.00 | 10.52 |
| ATOM | 1952 | SD  | MET | 325 | 63.227 | 78.025 | 77.440 | 1.00 | 13.36 |
| ATOM | 1953 | CE  | MET | 325 | 62.495 | 79.307 | 78.488 | 1.00 | 7.16  |
| ATOM | 1954 | C   | MET | 325 | 64.829 | 74.561 | 80.130 | 1.00 | 15.26 |
| ATOM | 1955 | O   | MET | 325 | 64.051 | 73.781 | 79.563 | 1.00 | 15.50 |
| ATOM | 1956 | N   | GLY | 326 | 64.848 | 74.751 | 81.447 | 1.00 | 15.85 |
| ATOM | 1957 | CA  | GLY | 326 | 63.899 | 74.093 | 82.323 | 1.00 | 17.08 |
| ATOM | 1958 | C   | GLY | 326 | 64.165 | 72.651 | 82.677 | 1.00 | 18.22 |
| ATOM | 1959 | O   | GLY | 326 | 63.270 | 71.957 | 83.148 | 1.00 | 18.82 |
| ATOM | 1960 | N   | CYS | 327 | 65.401 | 72.206 | 82.515 | 1.00 | 20.56 |
| ATOM | 1961 | CA  | CYS | 327 | 65.746 | 70.823 | 82.821 | 1.00 | 22.33 |
| ATOM | 1962 | CB  | CYS | 327 | 66.443 | 70.194 | 81.622 | 1.00 | 20.50 |
| ATOM | 1963 | SG  | CYS | 327 | 67.878 | 71.121 | 81.089 | 1.00 | 21.45 |
| ATOM | 1964 | C   | CYS | 327 | 66.633 | 70.710 | 84.061 | 1.00 | 24.86 |
| ATOM | 1965 | O   | CYS | 327 | 66.992 | 69.597 | 84.487 | 1.00 | 26.55 |
| ATOM | 1966 | N   | GLY | 328 | 67.007 | 71.859 | 84.619 | 1.00 | 23.64 |
| ATOM | 1967 | CA  | GLY | 328 | 67.846 | 71.867 | 85.802 | 1.00 | 23.90 |
| ATOM | 1968 | C   | GLY | 328 | 67.066 | 71.347 | 86.988 | 1.00 | 23.07 |
| ATOM | 1969 | O   | GLY | 328 | 65.913 | 71.735 | 87.168 | 1.00 | 23.22 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1970 | N   | SER | 329 | 67.706 | 70.528 | 87.822 | 1.00 | 23.68 |
| ATOM | 1971 | CA  | SER | 329 | 67.077 | 69.925 | 89.000 | 1.00 | 22.19 |
| ATOM | 1972 | CB  | SER | 329 | 68.150 | 69.406 | 89.964 | 1.00 | 19.55 |
| ATOM | 1973 | OG  | SER | 329 | 69.028 | 70.440 | 90.356 | 1.00 | 23.14 |
| ATOM | 1974 | C   | SER | 329 | 66.077 | 70.812 | 89.747 | 1.00 | 23.28 |
| ATOM | 1975 | O   | SER | 329 | 64.978 | 70.362 | 90.065 | 1.00 | 25.72 |
| ATOM | 1976 | N   | ILE | 330 | 66.444 | 72.070 | 89.992 | 1.00 | 22.81 |
| ATOM | 1977 | CA  | ILE | 330 | 65.584 | 73.024 | 90.700 | 1.00 | 19.85 |
| ATOM | 1978 | CB  | ILE | 330 | 66.410 | 74.017 | 91.589 | 1.00 | 15.67 |
| ATOM | 1979 | CG2 | ILE | 330 | 66.509 | 73.500 | 93.001 | 1.00 | 18.25 |
| ATOM | 1980 | CG1 | ILE | 330 | 67.795 | 74.289 | 90.994 | 1.00 | 7.11  |
| ATOM | 1981 | CD1 | ILE | 330 | 67.776 | 74.921 | 89.639 | 1.00 | 5.46  |
| ATOM | 1982 | C   | ILE | 330 | 64.703 | 73.869 | 89.786 | 1.00 | 20.60 |
| ATOM | 1983 | O   | ILE | 330 | 64.225 | 74.923 | 90.201 | 1.00 | 23.53 |
| ATOM | 1984 | N   | IMP | 331 | 64.425 | 73.400 | 88.579 | 1.00 | 19.32 |
| ATOM | 1985 | CA  | IMP | 331 | 63.641 | 74.206 | 87.649 | 1.00 | 20.33 |
| ATOM | 1986 | C   | IMP | 331 | 62.148 | 73.909 | 87.498 | 1.00 | 21.39 |
| ATOM | 1987 | O   | IMP | 331 | 61.737 | 72.757 | 87.342 | 1.00 | 22.62 |
| ATOM | 1988 | CB  | IMP | 331 | 64.310 | 74.200 | 86.277 | 1.00 | 19.26 |
| ATOM | 1989 | SG  | IMP | 331 | 64.038 | 75.775 | 85.516 | 1.00 | 16.83 |
| ATOM | 1990 | P   | IMP | 331 | 71.205 | 71.206 | 87.339 | 1.00 | 24.40 |
| ATOM | 1991 | O1P | IMP | 331 | 70.381 | 70.028 | 86.885 | 1.00 | 22.40 |
| ATOM | 1992 | O2P | IMP | 331 | 72.615 | 71.144 | 86.864 | 1.00 | 18.66 |
| ATOM | 1993 | O3P | IMP | 331 | 71.172 | 71.333 | 88.803 | 1.00 | 19.75 |
| ATOM | 1994 | O5* | IMP | 331 | 70.688 | 72.534 | 86.798 | 1.00 | 22.96 |
| ATOM | 1995 | C5* | IMP | 331 | 71.500 | 73.726 | 87.024 | 1.00 | 14.95 |
| ATOM | 1996 | C4* | IMP | 331 | 71.156 | 74.601 | 85.831 | 1.00 | 11.32 |
| ATOM | 1997 | O4* | IMP | 331 | 69.758 | 74.898 | 85.861 | 1.00 | 12.20 |
| ATOM | 1998 | C3* | IMP | 331 | 71.865 | 75.962 | 85.934 | 1.00 | 12.62 |
| ATOM | 1999 | O3* | IMP | 331 | 73.078 | 76.011 | 85.208 | 1.00 | 10.24 |
| ATOM | 2000 | C2* | IMP | 331 | 70.883 | 76.903 | 85.210 | 1.00 | 13.74 |
| ATOM | 2001 | O2* | IMP | 331 | 70.752 | 76.706 | 83.816 | 1.00 | 11.66 |
| ATOM | 2002 | C1* | IMP | 331 | 69.602 | 76.308 | 85.761 | 1.00 | 14.52 |
| ATOM | 2003 | N9  | IMP | 331 | 68.832 | 77.205 | 86.612 | 1.00 | 18.13 |
| ATOM | 2004 | C8  | IMP | 331 | 69.321 | 78.030 | 87.599 | 1.00 | 18.02 |
| ATOM | 2005 | N7  | IMP | 331 | 68.331 | 78.568 | 88.322 | 1.00 | 16.06 |
| ATOM | 2006 | C5  | IMP | 331 | 67.170 | 78.093 | 87.806 | 1.00 | 19.77 |
| ATOM | 2007 | C6  | IMP | 331 | 65.799 | 78.289 | 88.156 | 1.00 | 22.26 |
| ATOM | 2008 | O6  | IMP | 331 | 65.412 | 78.995 | 89.085 | 1.00 | 17.37 |
| ATOM | 2009 | N1  | IMP | 331 | 64.941 | 77.579 | 87.374 | 1.00 | 25.96 |
| ATOM | 2010 | C2  | IMP | 331 | 65.296 | 76.706 | 86.299 | 1.00 | 23.29 |
| ATOM | 2011 | N3  | IMP | 331 | 66.567 | 76.524 | 85.957 | 1.00 | 24.20 |
| ATOM | 2012 | C4  | IMP | 331 | 67.498 | 77.200 | 86.693 | 1.00 | 21.15 |
| ATOM | 2013 | N   | ILE | 332 | 61.333 | 74.959 | 87.564 | 1.00 | 19.04 |
| ATOM | 2014 | CA  | ILE | 332 | 59.899 | 74.811 | 87.391 | 1.00 | 18.02 |
| ATOM | 2015 | CB  | ILE | 332 | 59.071 | 75.097 | 88.696 | 1.00 | 16.99 |
| ATOM | 2016 | CG2 | ILE | 332 | 59.423 | 74.093 | 89.793 | 1.00 | 12.90 |
| ATOM | 2017 | CG1 | ILE | 332 | 59.283 | 76.525 | 89.191 | 1.00 | 14.79 |
| ATOM | 2018 | CD1 | ILE | 332 | 58.212 | 77.005 | 90.159 | 1.00 | 8.04  |
| ATOM | 2019 | C   | ILE | 332 | 59.401 | 75.675 | 86.226 | 1.00 | 20.21 |
| ATOM | 2020 | O   | ILE | 332 | 58.195 | 75.848 | 86.050 | 1.00 | 21.52 |
| ATOM | 2021 | N   | THR | 333 | 60.330 | 76.195 | 85.420 | 1.00 | 20.15 |
| ATOM | 2022 | CA  | THR | 333 | 59.993 | 77.020 | 84.251 | 1.00 | 19.79 |
| ATOM | 2023 | CB  | THR | 333 | 61.287 | 77.491 | 83.467 | 1.00 | 20.47 |
| ATOM | 2024 | OG1 | THR | 333 | 61.948 | 78.537 | 84.191 | 1.00 | 18.21 |
| ATOM | 2025 | CG2 | THR | 333 | 60.949 | 77.996 | 82.058 | 1.00 | 16.88 |
| ATOM | 2026 | C   | THR | 333 | 59.060 | 76.275 | 83.281 | 1.00 | 18.99 |
| ATOM | 2027 | O   | THR | 333 | 58.124 | 76.861 | 82.737 | 1.00 | 19.34 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2028 | N   | GLN | 334 | 59.308 | 74.988 | 83.063 | 1.00 | 16.88 |
| ATOM | 2029 | CA  | GLN | 334 | 58.469 | 74.229 | 82.150 | 1.00 | 16.64 |
| ATOM | 2030 | CB  | GLN | 334 | 59.077 | 72.850 | 81.863 | 1.00 | 15.49 |
| ATOM | 2031 | CG  | GLN | 334 | 60.004 | 72.864 | 80.658 | 1.00 | 16.53 |
| ATOM | 2032 | CD  | GLN | 334 | 60.874 | 71.628 | 80.536 | 1.00 | 18.34 |
| ATOM | 2033 | OE1 | GLN | 334 | 62.091 | 71.729 | 80.344 | 1.00 | 16.42 |
| ATOM | 2034 | NE2 | GLN | 334 | 60.257 | 70.461 | 80.604 | 1.00 | 20.90 |
| ATOM | 2035 | C   | GLN | 334 | 57.046 | 74.122 | 82.667 | 1.00 | 16.88 |
| ATOM | 2036 | O   | GLN | 334 | 56.091 | 74.293 | 81.916 | 1.00 | 15.78 |
| ATOM | 2037 | N   | GLU | 335 | 56.910 | 73.919 | 83.971 | 1.00 | 19.92 |
| ATOM | 2038 | CA  | GLU | 335 | 55.596 | 73.795 | 84.583 | 1.00 | 21.69 |
| ATOM | 2039 | CB  | GLU | 335 | 55.699 | 73.203 | 85.987 | 1.00 | 25.79 |
| ATOM | 2040 | CG  | GLU | 335 | 56.398 | 71.865 | 86.047 | 1.00 | 32.28 |
| ATOM | 2041 | CD  | GLU | 335 | 57.745 | 71.971 | 86.700 | 1.00 | 37.56 |
| ATOM | 2042 | OE1 | GLU | 335 | 58.715 | 72.312 | 85.988 | 1.00 | 35.47 |
| ATOM | 2043 | OE2 | GLU | 335 | 57.826 | 71.736 | 87.930 | 1.00 | 40.35 |
| ATOM | 2044 | C   | GLU | 335 | 54.878 | 75.123 | 84.675 | 1.00 | 20.91 |
| ATOM | 2045 | O   | GLU | 335 | 53.680 | 75.192 | 84.440 | 1.00 | 23.86 |
| ATOM | 2046 | N   | VAL | 336 | 55.608 | 76.176 | 85.022 | 1.00 | 20.29 |
| ATOM | 2047 | CA  | VAL | 336 | 55.003 | 77.488 | 85.167 | 1.00 | 18.99 |
| ATOM | 2048 | CB  | VAL | 336 | 55.776 | 78.368 | 86.175 | 1.00 | 19.44 |
| ATOM | 2049 | CG1 | VAL | 336 | 55.043 | 79.675 | 86.381 | 1.00 | 23.03 |
| ATOM | 2050 | CG2 | VAL | 336 | 55.922 | 77.651 | 87.510 | 1.00 | 16.34 |
| ATOM | 2051 | C   | VAL | 336 | 54.822 | 78.232 | 83.851 | 1.00 | 16.99 |
| ATOM | 2052 | O   | VAL | 336 | 53.752 | 78.764 | 83.595 | 1.00 | 17.91 |
| ATOM | 2053 | N   | LEU | 337 | 55.837 | 78.239 | 82.997 | 1.00 | 14.89 |
| ATOM | 2054 | CA  | LEU | 337 | 55.720 | 78.960 | 81.732 | 1.00 | 15.59 |
| ATOM | 2055 | CB  | LEU | 337 | 56.918 | 79.902 | 81.534 | 1.00 | 14.85 |
| ATOM | 2056 | CG  | LEU | 337 | 57.263 | 80.856 | 82.688 | 1.00 | 13.73 |
| ATOM | 2057 | CD1 | LEU | 337 | 58.394 | 81.763 | 82.271 | 1.00 | 14.07 |
| ATOM | 2058 | CD2 | LEU | 337 | 56.062 | 81.687 | 83.108 | 1.00 | 13.59 |
| ATOM | 2059 | C   | LEU | 337 | 55.468 | 78.133 | 80.467 | 1.00 | 14.97 |
| ATOM | 2060 | O   | LEU | 337 | 55.399 | 78.690 | 79.371 | 1.00 | 16.68 |
| ATOM | 2061 | N   | ALA | 338 | 55.386 | 76.812 | 80.599 | 1.00 | 12.41 |
| ATOM | 2062 | CA  | ALA | 338 | 55.109 | 75.933 | 79.456 | 1.00 | 12.62 |
| ATOM | 2063 | CB  | ALA | 338 | 53.732 | 76.248 | 78.887 | 1.00 | 13.39 |
| ATOM | 2064 | C   | ALA | 338 | 56.151 | 75.975 | 78.341 | 1.00 | 12.44 |
| ATOM | 2065 | O   | ALA | 338 | 55.996 | 75.339 | 77.289 | 1.00 | 9.63  |
| ATOM | 2066 | N   | CYS | 339 | 57.258 | 76.644 | 78.613 | 1.00 | 13.50 |
| ATOM | 2067 | CA  | CYS | 339 | 58.298 | 76.791 | 77.622 | 1.00 | 15.19 |
| ATOM | 2068 | CB  | CYS | 339 | 58.576 | 78.271 | 77.418 | 1.00 | 15.68 |
| ATOM | 2069 | SG  | CYS | 339 | 59.263 | 78.657 | 75.830 | 1.00 | 27.20 |
| ATOM | 2070 | C   | CYS | 339 | 59.558 | 76.077 | 78.057 | 1.00 | 16.02 |
| ATOM | 2071 | O   | CYS | 339 | 59.891 | 76.073 | 79.247 | 1.00 | 17.04 |
| ATOM | 2072 | N   | GLY | 340 | 60.249 | 75.480 | 77.086 | 1.00 | 14.98 |
| ATOM | 2073 | CA  | GLY | 340 | 61.480 | 74.759 | 77.355 | 1.00 | 11.03 |
| ATOM | 2074 | C   | GLY | 340 | 61.656 | 73.698 | 76.292 | 1.00 | 10.00 |
| ATOM | 2075 | O   | GLY | 340 | 60.972 | 73.741 | 75.267 | 1.00 | 9.29  |
| ATOM | 2076 | N   | ARG | 341 | 62.555 | 72.746 | 76.530 | 1.00 | 8.77  |
| ATOM | 2077 | CA  | ARG | 341 | 62.802 | 71.656 | 75.581 | 1.00 | 8.44  |
| ATOM | 2078 | CB  | ARG | 341 | 63.596 | 72.172 | 74.375 | 1.00 | 10.17 |
| ATOM | 2079 | CG  | ARG | 341 | 63.945 | 71.097 | 73.365 | 1.00 | 7.40  |
| ATOM | 2080 | CD  | ARG | 341 | 64.551 | 71.665 | 72.100 | 1.00 | 6.94  |
| ATOM | 2081 | NE  | ARG | 341 | 64.227 | 70.798 | 70.969 | 1.00 | 5.84  |
| ATOM | 2082 | CZ  | ARG | 341 | 64.577 | 71.034 | 69.712 | 1.00 | 2.98  |
| ATOM | 2083 | NH1 | ARG | 341 | 65.284 | 72.104 | 69.402 | 1.00 | 5.13  |
| ATOM | 2084 | NH2 | ARG | 341 | 64.143 | 70.240 | 68.750 | 1.00 | 5.18  |
| ATOM | 2085 | C   | ARG | 341 | 63.572 | 70.514 | 76.250 | 1.00 | 9.48  |

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FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2086 | O   | ARG | 341 | 64.384 | 70.756 | 77.140 | 1.00 | 10.70 |
| ATOM | 2087 | N   | PRO | 342 | 63.259 | 69.246 | 75.900 | 1.00 | 8.96  |
| ATOM | 2088 | CD  | PRO | 342 | 62.112 | 68.810 | 75.086 | 1.00 | 6.87  |
| ATOM | 2089 | CA  | PRO | 342 | 63.951 | 68.085 | 76.480 | 1.00 | 6.48  |
| ATOM | 2090 | CB  | PRO | 342 | 63.284 | 66.923 | 75.775 | 1.00 | 10.15 |
| ATOM | 2091 | CG  | PRO | 342 | 61.877 | 67.426 | 75.596 | 1.00 | 7.34  |
| ATOM | 2092 | C   | PRO | 342 | 65.446 | 68.168 | 76.164 | 1.00 | 8.19  |
| ATOM | 2093 | O   | PRO | 342 | 65.847 | 68.263 | 75.002 | 1.00 | 9.62  |
| ATOM | 2094 | N   | GLN | 343 | 66.267 | 68.096 | 77.206 | 1.00 | 9.33  |
| ATOM | 2095 | CA  | GLN | 343 | 67.706 | 68.262 | 77.080 | 1.00 | 10.57 |
| ATOM | 2096 | CB  | GLN | 343 | 68.385 | 68.138 | 78.440 | 1.00 | 11.05 |
| ATOM | 2097 | CG  | GLN | 343 | 69.766 | 68.799 | 78.495 | 1.00 | 10.72 |
| ATOM | 2098 | CD  | GLN | 343 | 69.749 | 70.264 | 78.090 | 1.00 | 16.93 |
| ATOM | 2099 | OE1 | GLN | 343 | 70.788 | 70.855 | 77.816 | 1.00 | 20.72 |
| ATOM | 2100 | NE2 | GLN | 343 | 68.571 | 70.865 | 78.082 | 1.00 | 20.86 |
| ATOM | 2101 | C   | GLN | 343 | 68.502 | 67.524 | 76.021 | 1.00 | 13.27 |
| ATOM | 2102 | O   | GLN | 343 | 69.166 | 68.160 | 75.202 | 1.00 | 15.52 |
| ATOM | 2103 | N   | ALA | 344 | 68.473 | 66.198 | 76.033 | 1.00 | 14.40 |
| ATOM | 2104 | CA  | ALA | 344 | 69.240 | 65.440 | 75.051 | 1.00 | 14.17 |
| ATOM | 2105 | CB  | ALA | 344 | 68.883 | 63.966 | 75.124 | 1.00 | 15.46 |
| ATOM | 2106 | C   | ALA | 344 | 69.011 | 65.983 | 73.643 | 1.00 | 14.10 |
| ATOM | 2107 | O   | ALA | 344 | 69.960 | 66.198 | 72.891 | 1.00 | 14.21 |
| ATOM | 2108 | N   | THR | 345 | 67.756 | 66.286 | 73.325 | 1.00 | 14.96 |
| ATOM | 2109 | CA  | THR | 345 | 67.413 | 66.801 | 72.008 | 1.00 | 13.41 |
| ATOM | 2110 | CB  | THR | 345 | 65.905 | 66.759 | 71.748 | 1.00 | 13.07 |
| ATOM | 2111 | OG1 | THR | 345 | 65.427 | 65.419 | 71.914 | 1.00 | 18.26 |
| ATOM | 2112 | CG2 | THR | 345 | 65.608 | 67.217 | 70.336 | 1.00 | 15.37 |
| ATOM | 2113 | C   | THR | 345 | 67.921 | 68.218 | 71.831 | 1.00 | 12.88 |
| ATOM | 2114 | O   | THR | 345 | 68.411 | 68.565 | 70.754 | 1.00 | 14.21 |
| ATOM | 2115 | N   | ALA | 346 | 67.811 | 69.033 | 72.880 | 1.00 | 11.75 |
| ATOM | 2116 | CA  | ALA | 346 | 68.286 | 70.418 | 72.817 | 1.00 | 9.99  |
| ATOM | 2117 | CB  | ALA | 346 | 68.032 | 71.126 | 74.126 | 1.00 | 6.11  |
| ATOM | 2118 | C   | ALA | 346 | 69.776 | 70.435 | 72.495 | 1.00 | 9.20  |
| ATOM | 2119 | O   | ALA | 346 | 70.218 | 71.139 | 71.600 | 1.00 | 11.48 |
| ATOM | 2120 | N   | VAL | 347 | 70.533 | 69.590 | 73.178 | 1.00 | 9.88  |
| ATOM | 2121 | CA  | VAL | 347 | 71.969 | 69.515 | 72.975 | 1.00 | 11.35 |
| ATOM | 2122 | CB  | VAL | 347 | 72.623 | 68.574 | 73.997 | 1.00 | 12.64 |
| ATOM | 2123 | CG1 | VAL | 347 | 74.106 | 68.431 | 73.701 | 1.00 | 12.61 |
| ATOM | 2124 | CG2 | VAL | 347 | 72.405 | 69.110 | 75.406 | 1.00 | 12.53 |
| ATOM | 2125 | C   | VAL | 347 | 72.372 | 69.091 | 71.571 | 1.00 | 12.67 |
| ATOM | 2126 | O   | VAL | 347 | 73.259 | 69.716 | 70.974 | 1.00 | 13.58 |
| ATOM | 2127 | N   | TYR | 348 | 71.738 | 68.044 | 71.042 | 1.00 | 11.86 |
| ATOM | 2128 | CA  | TYR | 348 | 72.071 | 67.559 | 69.707 | 1.00 | 9.76  |
| ATOM | 2129 | CB  | TYR | 348 | 71.371 | 66.235 | 69.408 | 1.00 | 9.26  |
| ATOM | 2130 | CG  | TYR | 348 | 71.466 | 65.839 | 67.953 | 1.00 | 10.84 |
| ATOM | 2131 | CD1 | TYR | 348 | 72.667 | 65.377 | 67.408 | 1.00 | 13.49 |
| ATOM | 2132 | CE1 | TYR | 348 | 72.776 | 65.071 | 66.042 | 1.00 | 14.55 |
| ATOM | 2133 | CD2 | TYR | 348 | 70.374 | 65.981 | 67.105 | 1.00 | 10.80 |
| ATOM | 2134 | CE2 | TYR | 348 | 70.469 | 65.682 | 65.748 | 1.00 | 12.01 |
| ATOM | 2135 | CZ  | TYR | 348 | 71.669 | 65.229 | 65.220 | 1.00 | 14.93 |
| ATOM | 2136 | OH  | TYR | 348 | 71.751 | 64.947 | 63.872 | 1.00 | 15.11 |
| ATOM | 2137 | C   | TYR | 348 | 71.735 | 68.567 | 68.620 | 1.00 | 12.81 |
| ATOM | 2138 | O   | TYR | 348 | 72.572 | 68.878 | 67.777 | 1.00 | 14.63 |
| ATOM | 2139 | N   | LYS | 349 | 70.508 | 69.076 | 68.630 | 1.00 | 13.27 |
| ATOM | 2140 | CA  | LYS | 349 | 70.081 | 70.043 | 67.622 | 1.00 | 14.33 |
| ATOM | 2141 | CB  | LYS | 349 | 68.596 | 70.349 | 67.792 | 1.00 | 16.10 |
| ATOM | 2142 | CG  | LYS | 349 | 67.689 | 69.177 | 67.466 | 1.00 | 19.74 |
| ATOM | 2143 | CD  | LYS | 349 | 67.707 | 68.886 | 65.974 | 1.00 | 25.23 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2144 | CE  | LYS | 349 | 66.783 | 67.735 | 65.626 | 1.00 | 32.56 |
| ATOM | 2145 | NZ  | LYS | 349 | 65.343 | 68.000 | 65.941 | 1.00 | 40.46 |
| ATOM | 2146 | C   | LYS | 349 | 70.877 | 71.352 | 67.537 | 1.00 | 15.33 |
| ATOM | 2147 | O   | LYS | 349 | 71.183 | 71.821 | 66.440 | 1.00 | 17.10 |
| ATOM | 2148 | N   | VAL | 350 | 71.206 | 71.953 | 68.676 | 1.00 | 15.15 |
| ATOM | 2149 | CA  | VAL | 350 | 71.937 | 73.214 | 68.662 | 1.00 | 14.07 |
| ATOM | 2150 | CB  | VAL | 350 | 71.794 | 73.992 | 69.989 | 1.00 | 14.19 |
| ATOM | 2151 | CG1 | VAL | 350 | 72.362 | 75.386 | 69.838 | 1.00 | 11.97 |
| ATOM | 2152 | CG2 | VAL | 350 | 70.337 | 74.078 | 70.392 | 1.00 | 17.18 |
| ATOM | 2153 | C   | VAL | 350 | 73.406 | 73.019 | 68.349 | 1.00 | 16.29 |
| ATOM | 2154 | O   | VAL | 350 | 73.995 | 73.838 | 67.645 | 1.00 | 18.00 |
| ATOM | 2155 | N   | SER | 351 | 74.006 | 71.958 | 68.886 | 1.00 | 16.00 |
| ATOM | 2156 | CA  | SER | 351 | 75.418 | 71.663 | 68.637 | 1.00 | 12.71 |
| ATOM | 2157 | CB  | SER | 351 | 75.882 | 70.505 | 69.517 | 1.00 | 11.95 |
| ATOM | 2158 | OG  | SER | 351 | 75.765 | 70.816 | 70.894 | 1.00 | 11.62 |
| ATOM | 2159 | C   | SER | 351 | 75.636 | 71.308 | 67.168 | 1.00 | 12.57 |
| ATOM | 2160 | O   | SER | 351 | 76.627 | 71.708 | 66.558 | 1.00 | 12.81 |
| ATOM | 2161 | N   | GLU | 352 | 74.698 | 70.556 | 66.606 | 1.00 | 13.06 |
| ATOM | 2162 | CA  | GLU | 352 | 74.770 | 70.152 | 65.219 | 1.00 | 12.95 |
| ATOM | 2163 | CB  | GLU | 352 | 73.565 | 69.292 | 64.887 | 1.00 | 14.63 |
| ATOM | 2164 | CG  | GLU | 352 | 73.753 | 68.340 | 63.728 | 1.00 | 24.19 |
| ATOM | 2165 | CD  | GLU | 352 | 73.820 | 69.039 | 62.393 | 1.00 | 31.22 |
| ATOM | 2166 | OE1 | GLU | 352 | 73.003 | 69.956 | 62.165 | 1.00 | 41.17 |
| ATOM | 2167 | OE2 | GLU | 352 | 74.688 | 68.677 | 61.569 | 1.00 | 31.62 |
| ATOM | 2168 | C   | GLU | 352 | 74.805 | 71.404 | 64.349 | 1.00 | 15.08 |
| ATOM | 2169 | O   | GLU | 352 | 75.499 | 71.434 | 63.339 | 1.00 | 19.18 |
| ATOM | 2170 | N   | TYR | 353 | 74.089 | 72.446 | 64.770 | 1.00 | 15.73 |
| ATOM | 2171 | CA  | TYR | 353 | 74.032 | 73.725 | 64.046 | 1.00 | 16.16 |
| ATOM | 2172 | CB  | TYR | 353 | 72.735 | 74.473 | 64.395 | 1.00 | 16.64 |
| ATOM | 2173 | CG  | TYR | 353 | 72.674 | 75.902 | 63.885 | 1.00 | 17.24 |
| ATOM | 2174 | CD1 | TYR | 353 | 72.487 | 76.171 | 62.535 | 1.00 | 17.57 |
| ATOM | 2175 | CE1 | TYR | 353 | 72.440 | 77.477 | 62.060 | 1.00 | 19.38 |
| ATOM | 2176 | CD2 | TYR | 353 | 72.810 | 76.986 | 64.756 | 1.00 | 20.21 |
| ATOM | 2177 | CE2 | TYR | 353 | 72.769 | 78.298 | 64.290 | 1.00 | 18.45 |
| ATOM | 2178 | CZ  | TYR | 353 | 72.580 | 78.534 | 62.941 | 1.00 | 21.67 |
| ATOM | 2179 | OH  | TYR | 353 | 72.534 | 79.821 | 62.458 | 1.00 | 26.08 |
| ATOM | 2180 | C   | TYR | 353 | 75.228 | 74.638 | 64.346 | 1.00 | 17.36 |
| ATOM | 2181 | O   | TYR | 353 | 75.930 | 75.099 | 63.438 | 1.00 | 16.84 |
| ATOM | 2182 | N   | ALA | 354 | 75.436 | 74.904 | 65.631 | 1.00 | 16.45 |
| ATOM | 2183 | CA  | ALA | 354 | 76.503 | 75.771 | 66.107 | 1.00 | 14.66 |
| ATOM | 2184 | CB  | ALA | 354 | 76.450 | 75.861 | 67.626 | 1.00 | 12.08 |
| ATOM | 2185 | C   | ALA | 354 | 77.881 | 75.327 | 65.649 | 1.00 | 15.93 |
| ATOM | 2186 | O   | ALA | 354 | 78.791 | 76.150 | 65.502 | 1.00 | 17.40 |
| ATOM | 2187 | N   | ARG | 355 | 78.044 | 74.029 | 65.412 | 1.00 | 16.56 |
| ATOM | 2188 | CA  | ARG | 355 | 79.331 | 73.503 | 64.974 | 1.00 | 15.93 |
| ATOM | 2189 | CB  | ARG | 355 | 79.327 | 71.972 | 64.970 | 1.00 | 12.81 |
| ATOM | 2190 | CG  | ARG | 355 | 78.353 | 71.355 | 64.005 | 1.00 | 13.40 |
| ATOM | 2191 | CD  | ARG | 355 | 78.750 | 69.953 | 63.679 | 1.00 | 10.78 |
| ATOM | 2192 | NE  | ARG | 355 | 77.902 | 69.377 | 62.648 | 1.00 | 11.50 |
| ATOM | 2193 | CZ  | ARG | 355 | 78.284 | 68.384 | 61.853 | 1.00 | 15.77 |
| ATOM | 2194 | NH1 | ARG | 355 | 79.500 | 67.863 | 61.977 | 1.00 | 20.37 |
| ATOM | 2195 | NH2 | ARG | 355 | 77.459 | 67.906 | 60.933 | 1.00 | 13.86 |
| ATOM | 2196 | C   | ARG | 355 | 79.719 | 74.024 | 63.594 | 1.00 | 16.63 |
| ATOM | 2197 | O   | ARG | 355 | 80.897 | 74.184 | 63.304 | 1.00 | 18.62 |
| ATOM | 2198 | N   | ARG | 356 | 78.727 | 74.340 | 62.768 | 1.00 | 17.13 |
| ATOM | 2199 | CA  | ARG | 356 | 78.980 | 74.844 | 61.424 | 1.00 | 18.61 |
| ATOM | 2200 | CB  | ARG | 356 | 77.694 | 74.786 | 60.591 | 1.00 | 20.45 |
| ATOM | 2201 | CG  | ARG | 356 | 76.842 | 73.548 | 60.869 | 1.00 | 26.84 |

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FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2202 | CD  | ARG | 356 | 75.749 | 73.356 | 59.835 | 1.00 | 35.30 |
| ATOM | 2203 | NE  | ARG | 356 | 76.289 | 72.781 | 58.600 | 1.00 | 45.31 |
| ATOM | 2204 | CZ  | ARG | 356 | 76.031 | 71.549 | 58.155 | 1.00 | 44.56 |
| ATOM | 2205 | NH1 | ARG | 356 | 75.228 | 70.736 | 58.839 | 1.00 | 41.95 |
| ATOM | 2206 | NH2 | ARG | 356 | 76.575 | 71.131 | 57.015 | 1.00 | 42.41 |
| ATOM | 2207 | C   | ARG | 356 | 79.518 | 76.277 | 61.478 | 1.00 | 20.86 |
| ATOM | 2208 | O   | ARG | 356 | 79.804 | 76.885 | 60.446 | 1.00 | 22.43 |
| ATOM | 2209 | N   | PHE | 357 | 79.651 | 76.816 | 62.687 | 1.00 | 21.28 |
| ATOM | 2210 | CA  | PHE | 357 | 80.157 | 78.170 | 62.885 | 1.00 | 19.44 |
| ATOM | 2211 | CB  | PHE | 357 | 79.031 | 79.081 | 63.369 | 1.00 | 17.23 |
| ATOM | 2212 | CG  | PHE | 357 | 77.830 | 79.068 | 62.481 | 1.00 | 17.05 |
| ATOM | 2213 | CD1 | PHE | 357 | 76.836 | 78.119 | 62.654 | 1.00 | 19.73 |
| ATOM | 2214 | CD2 | PHE | 357 | 77.712 | 79.977 | 61.439 | 1.00 | 18.18 |
| ATOM | 2215 | CE1 | PHE | 357 | 75.744 | 78.073 | 61.805 | 1.00 | 21.80 |
| ATOM | 2216 | CE2 | PHE | 357 | 76.619 | 79.940 | 60.583 | 1.00 | 19.81 |
| ATOM | 2217 | CZ  | PHE | 357 | 75.635 | 78.986 | 60.764 | 1.00 | 20.74 |
| ATOM | 2218 | C   | PHE | 357 | 81.270 | 78.145 | 63.917 | 1.00 | 20.90 |
| ATOM | 2219 | O   | PHE | 357 | 81.695 | 79.188 | 64.413 | 1.00 | 23.81 |
| ATOM | 2220 | N   | GLY | 358 | 81.725 | 76.944 | 64.250 | 1.00 | 20.23 |
| ATOM | 2221 | CA  | GLY | 358 | 82.782 | 76.794 | 65.230 | 1.00 | 21.34 |
| ATOM | 2222 | C   | GLY | 358 | 82.440 | 77.326 | 66.609 | 1.00 | 22.66 |
| ATOM | 2223 | O   | GLY | 358 | 83.319 | 77.829 | 67.308 | 1.00 | 25.20 |
| ATOM | 2224 | N   | VAL | 359 | 81.172 | 77.235 | 67.009 | 1.00 | 23.04 |
| ATOM | 2225 | CA  | VAL | 359 | 80.771 | 77.720 | 68.324 | 1.00 | 19.49 |
| ATOM | 2226 | CB  | VAL | 359 | 79.551 | 78.656 | 68.252 | 1.00 | 18.13 |
| ATOM | 2227 | CG1 | VAL | 359 | 79.241 | 79.201 | 69.620 | 1.00 | 17.64 |
| ATOM | 2228 | CG2 | VAL | 359 | 79.821 | 79.803 | 67.306 | 1.00 | 20.63 |
| ATOM | 2229 | C   | VAL | 359 | 80.472 | 76.555 | 69.262 | 1.00 | 17.44 |
| ATOM | 2230 | O   | VAL | 359 | 79.623 | 75.710 | 68.982 | 1.00 | 18.55 |
| ATOM | 2231 | N   | PRO | 360 | 81.251 | 76.441 | 70.341 | 1.00 | 15.36 |
| ATOM | 2232 | CD  | PRO | 360 | 82.498 | 77.197 | 70.545 | 1.00 | 11.72 |
| ATOM | 2233 | CA  | PRO | 360 | 81.108 | 75.392 | 71.353 | 1.00 | 14.20 |
| ATOM | 2234 | CB  | PRO | 360 | 82.273 | 75.679 | 72.298 | 1.00 | 11.22 |
| ATOM | 2235 | CG  | PRO | 360 | 83.302 | 76.259 | 71.388 | 1.00 | 11.79 |
| ATOM | 2236 | C   | PRO | 360 | 79.774 | 75.498 | 72.096 | 1.00 | 14.81 |
| ATOM | 2237 | O   | PRO | 360 | 79.312 | 76.602 | 72.393 | 1.00 | 16.13 |
| ATOM | 2238 | N   | VAL | 361 | 79.153 | 74.355 | 72.372 | 1.00 | 13.23 |
| ATOM | 2239 | CA  | VAL | 361 | 77.892 | 74.313 | 73.099 | 1.00 | 9.02  |
| ATOM | 2240 | CB  | VAL | 361 | 76.849 | 73.453 | 72.362 | 1.00 | 6.35  |
| ATOM | 2241 | CG1 | VAL | 361 | 75.793 | 72.907 | 73.331 | 1.00 | 4.83  |
| ATOM | 2242 | CG2 | VAL | 361 | 76.175 | 74.289 | 71.286 | 1.00 | 9.33  |
| ATOM | 2243 | C   | VAL | 361 | 78.154 | 73.739 | 74.483 | 1.00 | 11.18 |
| ATOM | 2244 | O   | VAL | 361 | 78.917 | 72.775 | 74.623 | 1.00 | 12.24 |
| ATOM | 2245 | N   | ILE | 362 | 77.545 | 74.359 | 75.495 | 1.00 | 10.96 |
| ATOM | 2246 | CA  | ILE | 362 | 77.659 | 73.950 | 76.895 | 1.00 | 9.15  |
| ATOM | 2247 | CB  | ILE | 362 | 77.836 | 75.184 | 77.831 | 1.00 | 9.87  |
| ATOM | 2248 | CG2 | ILE | 362 | 77.850 | 74.769 | 79.294 | 1.00 | 5.57  |
| ATOM | 2249 | CG1 | ILE | 362 | 79.130 | 75.931 | 77.504 | 1.00 | 14.42 |
| ATOM | 2250 | CD1 | ILE | 362 | 79.377 | 77.131 | 78.394 | 1.00 | 14.31 |
| ATOM | 2251 | C   | ILE | 362 | 76.345 | 73.283 | 77.263 | 1.00 | 9.83  |
| ATOM | 2252 | O   | ILE | 362 | 75.318 | 73.949 | 77.305 | 1.00 | 12.05 |
| ATOM | 2253 | N   | ALA | 363 | 76.357 | 71.972 | 77.485 | 1.00 | 11.91 |
| ATOM | 2254 | CA  | ALA | 363 | 75.136 | 71.256 | 77.868 | 1.00 | 11.28 |
| ATOM | 2255 | CB  | ALA | 363 | 75.319 | 69.763 | 77.724 | 1.00 | 13.29 |
| ATOM | 2256 | C   | ALA | 363 | 74.880 | 71.623 | 79.314 | 1.00 | 12.59 |
| ATOM | 2257 | O   | ALA | 363 | 75.519 | 71.100 | 80.231 | 1.00 | 14.94 |
| ATOM | 2258 | N   | ASP | 364 | 73.943 | 72.538 | 79.505 | 1.00 | 13.34 |
| ATOM | 2259 | CA  | ASP | 364 | 73.617 | 73.056 | 80.816 | 1.00 | 12.33 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2260 | CB  | ASP | 364 | 73.737 | 74.577 | 80.750 | 1.00 | 11.24 |
| ATOM | 2261 | CG  | ASP | 364 | 73.210 | 75.255 | 81.966 | 1.00 | 15.61 |
| ATOM | 2262 | OD1 | ASP | 364 | 73.322 | 74.677 | 83.061 | 1.00 | 18.33 |
| ATOM | 2263 | OD2 | ASP | 364 | 72.680 | 76.372 | 81.820 | 1.00 | 22.45 |
| ATOM | 2264 | C   | ASP | 364 | 72.257 | 72.630 | 81.371 | 1.00 | 14.11 |
| ATOM | 2265 | O   | ASP | 364 | 71.207 | 73.094 | 80.915 | 1.00 | 12.91 |
| ATOM | 2266 | N   | GLY | 365 | 72.294 | 71.795 | 82.409 | 1.00 | 15.80 |
| ATOM | 2267 | CA  | GLY | 365 | 71.068 | 71.324 | 83.036 | 1.00 | 17.03 |
| ATOM | 2268 | C   | GLY | 365 | 70.702 | 69.854 | 82.863 | 1.00 | 17.21 |
| ATOM | 2269 | O   | GLY | 365 | 70.933 | 69.257 | 81.807 | 1.00 | 16.26 |
| ATOM | 2270 | N   | GLY | 366 | 70.137 | 69.269 | 83.919 | 1.00 | 19.08 |
| ATOM | 2271 | CA  | GLY | 366 | 69.711 | 67.883 | 83.875 | 1.00 | 20.17 |
| ATOM | 2272 | C   | GLY | 366 | 70.777 | 66.832 | 84.104 | 1.00 | 21.83 |
| ATOM | 2273 | O   | GLY | 366 | 70.487 | 65.635 | 84.002 | 1.00 | 22.67 |
| ATOM | 2274 | N   | ILE | 367 | 72.009 | 67.253 | 84.384 | 1.00 | 22.88 |
| ATOM | 2275 | CA  | ILE | 367 | 73.098 | 66.311 | 84.634 | 1.00 | 22.10 |
| ATOM | 2276 | CB  | ILE | 367 | 74.484 | 66.959 | 84.444 | 1.00 | 20.00 |
| ATOM | 2277 | CG2 | ILE | 367 | 75.596 | 65.980 | 84.841 | 1.00 | 18.29 |
| ATOM | 2278 | CG1 | ILE | 367 | 74.643 | 67.462 | 83.002 | 1.00 | 18.25 |
| ATOM | 2279 | CD1 | ILE | 367 | 74.511 | 66.400 | 81.937 | 1.00 | 17.72 |
| ATOM | 2280 | C   | ILE | 367 | 72.975 | 65.803 | 86.063 | 1.00 | 24.54 |
| ATOM | 2281 | O   | ILE | 367 | 73.240 | 66.534 | 87.018 | 1.00 | 25.34 |
| ATOM | 2282 | N   | GLN | 368 | 72.533 | 64.559 | 86.198 | 1.00 | 25.47 |
| ATOM | 2283 | CA  | GLN | 368 | 72.352 | 63.929 | 87.500 | 1.00 | 26.05 |
| ATOM | 2284 | CB  | GLN | 368 | 71.010 | 63.193 | 87.546 | 1.00 | 33.00 |
| ATOM | 2285 | CG  | GLN | 368 | 69.808 | 63.960 | 87.016 | 1.00 | 41.39 |
| ATOM | 2286 | CD  | GLN | 368 | 68.650 | 63.034 | 86.645 | 1.00 | 47.49 |
| ATOM | 2287 | OE1 | GLN | 368 | 68.857 | 61.864 | 86.306 | 1.00 | 50.05 |
| ATOM | 2288 | NE2 | GLN | 368 | 67.435 | 63.566 | 86.664 | 1.00 | 49.52 |
| ATOM | 2289 | C   | GLN | 368 | 73.462 | 62.923 | 87.807 | 1.00 | 23.20 |
| ATOM | 2290 | O   | GLN | 368 | 73.581 | 62.460 | 88.939 | 1.00 | 24.66 |
| ATOM | 2291 | N   | ASN | 369 | 74.249 | 62.558 | 86.797 | 1.00 | 20.24 |
| ATOM | 2292 | CA  | ASN | 369 | 75.322 | 61.586 | 86.979 | 1.00 | 17.49 |
| ATOM | 2293 | CB  | ASN | 369 | 74.721 | 60.205 | 87.203 | 1.00 | 18.55 |
| ATOM | 2294 | CG  | ASN | 369 | 73.906 | 59.736 | 86.025 | 1.00 | 19.68 |
| ATOM | 2295 | OD1 | ASN | 369 | 73.929 | 60.334 | 84.947 | 1.00 | 20.92 |
| ATOM | 2296 | ND2 | ASN | 369 | 73.182 | 58.654 | 86.217 | 1.00 | 27.57 |
| ATOM | 2297 | C   | ASN | 369 | 76.269 | 61.537 | 85.781 | 1.00 | 16.13 |
| ATOM | 2298 | O   | ASN | 369 | 76.062 | 62.238 | 84.790 | 1.00 | 16.39 |
| ATOM | 2299 | N   | VAL | 370 | 77.274 | 60.670 | 85.859 | 1.00 | 15.11 |
| ATOM | 2300 | CA  | VAL | 370 | 78.261 | 60.533 | 84.793 | 1.00 | 14.39 |
| ATOM | 2301 | CB  | VAL | 370 | 79.396 | 59.566 | 85.179 | 1.00 | 10.30 |
| ATOM | 2302 | CG1 | VAL | 370 | 80.297 | 59.311 | 83.984 | 1.00 | 14.21 |
| ATOM | 2303 | CG2 | VAL | 370 | 80.216 | 60.150 | 86.300 | 1.00 | 7.21  |
| ATOM | 2304 | C   | VAL | 370 | 77.693 | 60.122 | 83.438 | 1.00 | 16.18 |
| ATOM | 2305 | O   | VAL | 370 | 78.148 | 60.616 | 82.406 | 1.00 | 20.19 |
| ATOM | 2306 | N   | GLY | 371 | 76.702 | 59.238 | 83.429 | 1.00 | 15.14 |
| ATOM | 2307 | CA  | GLY | 371 | 76.125 | 58.802 | 82.170 | 1.00 | 12.93 |
| ATOM | 2308 | C   | GLY | 371 | 75.635 | 59.981 | 81.357 | 1.00 | 14.21 |
| ATOM | 2309 | O   | GLY | 371 | 75.845 | 60.052 | 80.144 | 1.00 | 16.14 |
| ATOM | 2310 | N   | HIS | 372 | 74.994 | 60.921 | 82.041 | 1.00 | 14.52 |
| ATOM | 2311 | CA  | HIS | 372 | 74.467 | 62.121 | 81.411 | 1.00 | 12.09 |
| ATOM | 2312 | CB  | HIS | 372 | 73.717 | 62.965 | 82.442 | 1.00 | 13.52 |
| ATOM | 2313 | CG  | HIS | 372 | 72.452 | 62.338 | 82.941 | 1.00 | 11.76 |
| ATOM | 2314 | CD2 | HIS | 372 | 71.675 | 62.637 | 84.006 | 1.00 | 9.64  |
| ATOM | 2315 | ND1 | HIS | 372 | 71.836 | 61.283 | 82.301 | 1.00 | 11.22 |
| ATOM | 2316 | CE1 | HIS | 372 | 70.730 | 60.964 | 82.950 | 1.00 | 11.70 |
| ATOM | 2317 | NE2 | HIS | 372 | 70.609 | 61.769 | 83.989 | 1.00 | 13.93 |



FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2318 | C   | HIS | 372 | 75.584 | 62.936 | 80.783 | 1.00 | 11.92 |
| ATOM | 2319 | O   | HIS | 372 | 75.477 | 63.351 | 79.633 | 1.00 | 13.70 |
| ATOM | 2320 | N   | ILE | 373 | 76.664 | 63.150 | 81.529 | 1.00 | 11.48 |
| ATOM | 2321 | CA  | ILE | 373 | 77.802 | 63.912 | 81.023 | 1.00 | 10.28 |
| ATOM | 2322 | CB  | ILE | 373 | 78.970 | 63.936 | 82.020 | 1.00 | 9.11  |
| ATOM | 2323 | CG2 | ILE | 373 | 80.052 | 64.869 | 81.511 | 1.00 | 9.72  |
| ATOM | 2324 | CG1 | ILE | 373 | 78.500 | 64.430 | 83.390 | 1.00 | 12.51 |
| ATOM | 2325 | CD1 | ILE | 373 | 79.615 | 64.553 | 84.422 | 1.00 | 7.16  |
| ATOM | 2326 | C   | ILE | 373 | 78.305 | 63.320 | 79.705 | 1.00 | 11.05 |
| ATOM | 2327 | O   | ILE | 373 | 78.401 | 64.023 | 78.696 | 1.00 | 13.77 |
| ATOM | 2328 | N   | ALA | 374 | 78.578 | 62.019 | 79.709 | 1.00 | 10.10 |
| ATOM | 2329 | CA  | ALA | 374 | 79.059 | 61.323 | 78.521 | 1.00 | 7.10  |
| ATOM | 2330 | CB  | ALA | 374 | 79.338 | 59.858 | 78.849 | 1.00 | 6.65  |
| ATOM | 2331 | C   | ALA | 374 | 78.077 | 61.436 | 77.354 | 1.00 | 7.00  |
| ATOM | 2332 | O   | ALA | 374 | 78.494 | 61.582 | 76.200 | 1.00 | 7.81  |
| ATOM | 2333 | N   | LYS | 375 | 76.779 | 61.375 | 77.649 | 1.00 | 6.65  |
| ATOM | 2334 | CA  | LYS | 375 | 75.747 | 61.485 | 76.618 | 1.00 | 7.92  |
| ATOM | 2335 | CB  | LYS | 375 | 74.372 | 61.114 | 77.168 | 1.00 | 10.47 |
| ATOM | 2336 | CG  | LYS | 375 | 74.227 | 59.656 | 77.562 | 1.00 | 12.38 |
| ATOM | 2337 | CD  | LYS | 375 | 72.820 | 59.354 | 78.030 | 1.00 | 9.26  |
| ATOM | 2338 | CE  | LYS | 375 | 72.730 | 57.927 | 78.518 | 1.00 | 7.92  |
| ATOM | 2339 | NZ  | LYS | 375 | 71.353 | 57.566 | 78.921 | 1.00 | 7.20  |
| ATOM | 2340 | C   | LYS | 375 | 75.680 | 62.885 | 76.021 | 1.00 | 9.52  |
| ATOM | 2341 | O   | LYS | 375 | 75.457 | 63.036 | 74.825 | 1.00 | 12.41 |
| ATOM | 2342 | N   | ALA | 376 | 75.847 | 63.911 | 76.850 | 1.00 | 8.56  |
| ATOM | 2343 | CA  | ALA | 376 | 75.819 | 65.286 | 76.359 | 1.00 | 8.01  |
| ATOM | 2344 | CB  | ALA | 376 | 75.989 | 66.258 | 77.505 | 1.00 | 6.06  |
| ATOM | 2345 | C   | ALA | 376 | 76.951 | 65.466 | 75.362 | 1.00 | 7.56  |
| ATOM | 2346 | O   | ALA | 376 | 76.755 | 65.969 | 74.261 | 1.00 | 6.99  |
| ATOM | 2347 | N   | LEU | 377 | 78.137 | 65.031 | 75.766 | 1.00 | 9.38  |
| ATOM | 2348 | CA  | LEU | 377 | 79.331 | 65.132 | 74.940 | 1.00 | 11.38 |
| ATOM | 2349 | CB  | LEU | 377 | 80.550 | 64.633 | 75.725 | 1.00 | 10.28 |
| ATOM | 2350 | CG  | LEU | 377 | 80.816 | 65.413 | 77.016 | 1.00 | 8.99  |
| ATOM | 2351 | CD1 | LEU | 377 | 81.864 | 64.704 | 77.875 | 1.00 | 8.49  |
| ATOM | 2352 | CD2 | LEU | 377 | 81.221 | 66.847 | 76.678 | 1.00 | 2.00  |
| ATOM | 2353 | C   | LEU | 377 | 79.168 | 64.354 | 73.644 | 1.00 | 12.35 |
| ATOM | 2354 | O   | LEU | 377 | 79.457 | 64.862 | 72.566 | 1.00 | 12.88 |
| ATOM | 2355 | N   | ALA | 378 | 78.660 | 63.132 | 73.755 | 1.00 | 15.20 |
| ATOM | 2356 | CA  | ALA | 378 | 78.436 | 62.270 | 72.598 | 1.00 | 14.02 |
| ATOM | 2357 | CB  | ALA | 378 | 77.927 | 60.907 | 73.057 | 1.00 | 12.75 |
| ATOM | 2358 | C   | ALA | 378 | 77.453 | 62.891 | 71.609 | 1.00 | 13.17 |
| ATOM | 2359 | O   | ALA | 378 | 77.501 | 62.601 | 70.419 | 1.00 | 16.35 |
| ATOM | 2360 | N   | LEU | 379 | 76.562 | 63.749 | 72.097 | 1.00 | 13.73 |
| ATOM | 2361 | CA  | LEU | 379 | 75.567 | 64.376 | 71.236 | 1.00 | 12.58 |
| ATOM | 2362 | CB  | LEU | 379 | 74.234 | 64.517 | 71.968 | 1.00 | 11.76 |
| ATOM | 2363 | CG  | LEU | 379 | 73.485 | 63.201 | 72.194 | 1.00 | 12.16 |
| ATOM | 2364 | CD1 | LEU | 379 | 72.225 | 63.447 | 72.983 | 1.00 | 11.41 |
| ATOM | 2365 | CD2 | LEU | 379 | 73.171 | 62.563 | 70.863 | 1.00 | 10.14 |
| ATOM | 2366 | C   | LEU | 379 | 75.980 | 65.706 | 70.621 | 1.00 | 14.62 |
| ATOM | 2367 | O   | LEU | 379 | 75.220 | 66.294 | 69.848 | 1.00 | 16.75 |
| ATOM | 2368 | N   | GLY | 380 | 77.175 | 66.183 | 70.950 | 1.00 | 14.81 |
| ATOM | 2369 | CA  | GLY | 380 | 77.636 | 67.427 | 70.371 | 1.00 | 12.86 |
| ATOM | 2370 | C   | GLY | 380 | 78.128 | 68.502 | 71.325 | 1.00 | 15.25 |
| ATOM | 2371 | O   | GLY | 380 | 78.734 | 69.476 | 70.869 | 1.00 | 17.13 |
| ATOM | 2372 | N   | ALA | 381 | 77.899 | 68.356 | 72.626 | 1.00 | 12.90 |
| ATOM | 2373 | CA  | ALA | 381 | 78.348 | 69.390 | 73.547 | 1.00 | 12.21 |
| ATOM | 2374 | CB  | ALA | 381 | 77.635 | 69.269 | 74.873 | 1.00 | 5.91  |
| ATOM | 2375 | C   | ALA | 381 | 79.862 | 69.368 | 73.744 | 1.00 | 16.09 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2376 | O   | ALA | 381 | 80.487 | 68.294 | 73.764 | 1.00 | 16.75 |
| ATOM | 2377 | N   | SER | 382 | 80.461 | 70.553 | 73.833 | 1.00 | 16.25 |
| ATOM | 2378 | CA  | SER | 382 | 81.898 | 70.647 | 74.050 | 1.00 | 14.46 |
| ATOM | 2379 | CB  | SER | 382 | 82.464 | 71.911 | 73.394 | 1.00 | 15.52 |
| ATOM | 2380 | OG  | SER | 382 | 82.399 | 71.835 | 71.978 | 1.00 | 12.28 |
| ATOM | 2381 | C   | SER | 382 | 82.223 | 70.612 | 75.545 | 1.00 | 12.47 |
| ATOM | 2382 | O   | SER | 382 | 83.293 | 70.160 | 75.946 | 1.00 | 12.89 |
| ATOM | 2383 | N   | THR | 383 | 81.299 | 71.093 | 76.363 | 1.00 | 9.47  |
| ATOM | 2384 | CA  | THR | 383 | 81.479 | 71.102 | 77.805 | 1.00 | 9.10  |
| ATOM | 2385 | CB  | THR | 383 | 82.060 | 72.464 | 78.312 | 1.00 | 9.34  |
| ATOM | 2386 | OG1 | THR | 383 | 81.386 | 73.555 | 77.677 | 1.00 | 7.51  |
| ATOM | 2387 | CG2 | THR | 383 | 83.552 | 72.573 | 78.009 | 1.00 | 9.52  |
| ATOM | 2388 | C   | THR | 383 | 80.122 | 70.814 | 78.452 | 1.00 | 9.96  |
| ATOM | 2389 | O   | THR | 383 | 79.100 | 70.808 | 77.768 | 1.00 | 11.79 |
| ATOM | 2390 | N   | VAL | 384 | 80.112 | 70.554 | 79.755 | 1.00 | 11.42 |
| ATOM | 2391 | CA  | VAL | 384 | 78.884 | 70.254 | 80.489 | 1.00 | 12.61 |
| ATOM | 2392 | CB  | VAL | 384 | 78.806 | 68.743 | 80.858 | 1.00 | 12.85 |
| ATOM | 2393 | CG1 | VAL | 384 | 77.655 | 68.485 | 81.816 | 1.00 | 9.44  |
| ATOM | 2394 | CG2 | VAL | 384 | 78.617 | 67.906 | 79.597 | 1.00 | 8.74  |
| ATOM | 2395 | C   | VAL | 384 | 78.867 | 71.083 | 81.766 | 1.00 | 13.72 |
| ATOM | 2396 | O   | VAL | 384 | 79.855 | 71.121 | 82.488 | 1.00 | 16.90 |
| ATOM | 2397 | N   | MET | 385 | 77.743 | 71.737 | 82.042 | 1.00 | 12.85 |
| ATOM | 2398 | CA  | MET | 385 | 77.603 | 72.568 | 83.235 | 1.00 | 11.55 |
| ATOM | 2399 | CB  | MET | 385 | 77.037 | 73.941 | 82.849 | 1.00 | 9.59  |
| ATOM | 2400 | CG  | MET | 385 | 76.925 | 74.933 | 83.997 | 1.00 | 8.37  |
| ATOM | 2401 | SD  | MET | 385 | 76.483 | 76.589 | 83.443 | 1.00 | 15.71 |
| ATOM | 2402 | CE  | MET | 385 | 78.077 | 77.210 | 82.918 | 1.00 | 11.94 |
| ATOM | 2403 | C   | MET | 385 | 76.682 | 71.874 | 84.232 | 1.00 | 13.51 |
| ATOM | 2404 | O   | MET | 385 | 75.617 | 71.391 | 83.855 | 1.00 | 16.34 |
| ATOM | 2405 | N   | MET | 386 | 77.092 | 71.818 | 85.494 | 1.00 | 13.54 |
| ATOM | 2406 | CA  | MET | 386 | 76.302 | 71.175 | 86.536 | 1.00 | 12.69 |
| ATOM | 2407 | CB  | MET | 386 | 77.046 | 69.970 | 87.093 | 1.00 | 11.47 |
| ATOM | 2408 | CG  | MET | 386 | 77.370 | 68.902 | 86.095 | 1.00 | 15.31 |
| ATOM | 2409 | SD  | MET | 386 | 79.102 | 68.453 | 86.167 | 1.00 | 23.72 |
| ATOM | 2410 | CE  | MET | 386 | 79.227 | 67.858 | 87.814 | 1.00 | 23.52 |
| ATOM | 2411 | C   | MET | 386 | 75.996 | 72.107 | 87.700 | 1.00 | 14.87 |
| ATOM | 2412 | O   | MET | 386 | 76.761 | 73.028 | 88.006 | 1.00 | 14.78 |
| ATOM | 2413 | N   | GLY | 387 | 74.881 | 71.836 | 88.366 | 1.00 | 16.33 |
| ATOM | 2414 | CA  | GLY | 387 | 74.471 | 72.615 | 89.517 | 1.00 | 16.37 |
| ATOM | 2415 | C   | GLY | 387 | 74.350 | 71.680 | 90.700 | 1.00 | 17.64 |
| ATOM | 2416 | O   | GLY | 387 | 75.172 | 71.725 | 91.611 | 1.00 | 18.53 |
| ATOM | 2417 | N   | SER | 388 | 73.389 | 70.762 | 90.650 | 1.00 | 18.70 |
| ATOM | 2418 | CA  | SER | 388 | 73.197 | 69.827 | 91.750 | 1.00 | 20.06 |
| ATOM | 2419 | CB  | SER | 388 | 71.854 | 69.094 | 91.646 | 1.00 | 19.62 |
| ATOM | 2420 | OG  | SER | 388 | 71.786 | 68.278 | 90.492 | 1.00 | 23.96 |
| ATOM | 2421 | C   | SER | 388 | 74.324 | 68.822 | 91.904 | 1.00 | 21.02 |
| ATOM | 2422 | O   | SER | 388 | 74.641 | 68.418 | 93.024 | 1.00 | 23.46 |
| ATOM | 2423 | N   | LEU | 389 | 74.967 | 68.452 | 90.804 | 1.00 | 20.62 |
| ATOM | 2424 | CA  | LEU | 389 | 76.048 | 67.475 | 90.873 | 1.00 | 19.98 |
| ATOM | 2425 | CB  | LEU | 389 | 76.388 | 66.931 | 89.479 | 1.00 | 16.24 |
| ATOM | 2426 | CG  | LEU | 389 | 76.903 | 65.485 | 89.459 | 1.00 | 12.91 |
| ATOM | 2427 | CD1 | LEU | 389 | 75.862 | 64.596 | 90.088 | 1.00 | 9.27  |
| ATOM | 2428 | CD2 | LEU | 389 | 77.207 | 65.012 | 88.053 | 1.00 | 7.57  |
| ATOM | 2429 | C   | LEU | 389 | 77.294 | 68.028 | 91.555 | 1.00 | 22.25 |
| ATOM | 2430 | O   | LEU | 389 | 78.297 | 67.335 | 91.656 | 1.00 | 24.36 |
| ATOM | 2431 | N   | LEU | 390 | 77.224 | 69.269 | 92.033 | 1.00 | 23.31 |
| ATOM | 2432 | CA  | LEU | 390 | 78.350 | 69.906 | 92.712 | 1.00 | 21.02 |
| ATOM | 2433 | CB  | LEU | 390 | 79.049 | 70.892 | 91.769 | 1.00 | 17.40 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2434 | CG  | LEU | 390 | 79.563 | 70.361 | 90.424  | 1.00 | 13.45 |
| ATOM | 2435 | CD1 | LEU | 390 | 80.108 | 71.494 | 89.584  | 1.00 | 11.98 |
| ATOM | 2436 | CD2 | LEU | 390 | 80.643 | 69.326 | 90.656  | 1.00 | 14.99 |
| ATOM | 2437 | C   | LEU | 390 | 77.886 | 70.651 | 93.963  | 1.00 | 22.78 |
| ATOM | 2438 | O   | LEU | 390 | 78.640 | 70.796 | 94.922  | 1.00 | 23.75 |
| ATOM | 2439 | N   | ALA | 391 | 76.624 | 71.066 | 93.965  | 1.00 | 25.01 |
| ATOM | 2440 | CA  | ALA | 391 | 76.020 | 71.827 | 95.061  | 1.00 | 27.66 |
| ATOM | 2441 | CB  | ALA | 391 | 74.513 | 71.970 | 94.832  | 1.00 | 24.32 |
| ATOM | 2442 | C   | ALA | 391 | 76.282 | 71.409 | 96.511  | 1.00 | 30.02 |
| ATOM | 2443 | O   | ALA | 391 | 76.112 | 72.227 | 97.422  | 1.00 | 33.60 |
| ATOM | 2444 | N   | ALA | 392 | 76.660 | 70.160 | 96.755  | 1.00 | 28.04 |
| ATOM | 2445 | CA  | ALA | 392 | 76.897 | 69.748 | 98.136  | 1.00 | 27.13 |
| ATOM | 2446 | CB  | ALA | 392 | 76.046 | 68.559 | 98.478  | 1.00 | 30.74 |
| ATOM | 2447 | C   | ALA | 392 | 78.348 | 69.453 | 98.461  | 1.00 | 25.59 |
| ATOM | 2448 | O   | ALA | 392 | 78.643 | 68.723 | 99.410  | 1.00 | 23.24 |
| ATOM | 2449 | N   | THR | 393 | 79.256 | 69.969 | 97.649  | 1.00 | 24.15 |
| ATOM | 2450 | CA  | THR | 393 | 80.663 | 69.734 | 97.895  | 1.00 | 22.30 |
| ATOM | 2451 | CB  | THR | 393 | 81.502 | 69.799 | 96.599  | 1.00 | 18.89 |
| ATOM | 2452 | OG1 | THR | 393 | 81.294 | 71.053 | 95.952  | 1.00 | 21.65 |
| ATOM | 2453 | CG2 | THR | 393 | 81.121 | 68.666 | 95.651  | 1.00 | 15.42 |
| ATOM | 2454 | C   | THR | 393 | 81.162 | 70.760 | 98.894  | 1.00 | 23.37 |
| ATOM | 2455 | O   | THR | 393 | 80.514 | 71.781 | 99.133  | 1.00 | 23.21 |
| ATOM | 2456 | N   | THR | 394 | 82.316 | 70.475 | 99.481  | 1.00 | 23.31 |
| ATOM | 2457 | CA  | THR | 394 | 82.927 | 71.349 | 100.471 | 1.00 | 22.67 |
| ATOM | 2458 | CB  | THR | 394 | 84.257 | 70.731 | 100.977 | 1.00 | 25.02 |
| ATOM | 2459 | OG1 | THR | 394 | 84.042 | 69.352 | 101.309 | 1.00 | 27.81 |
| ATOM | 2460 | CG2 | THR | 394 | 84.761 | 71.462 | 102.215 | 1.00 | 25.38 |
| ATOM | 2461 | C   | THR | 394 | 83.206 | 72.756 | 99.933  | 1.00 | 20.08 |
| ATOM | 2462 | O   | THR | 394 | 83.028 | 73.743 | 100.636 | 1.00 | 21.25 |
| ATOM | 2463 | N   | GLU | 395 | 83.589 | 72.843 | 98.667  | 1.00 | 17.87 |
| ATOM | 2464 | CA  | GLU | 395 | 83.935 | 74.115 | 98.066  | 1.00 | 15.59 |
| ATOM | 2465 | CB  | GLU | 395 | 84.879 | 73.906 | 96.887  | 1.00 | 18.03 |
| ATOM | 2466 | CG  | GLU | 395 | 86.264 | 73.351 | 97.255  | 1.00 | 21.45 |
| ATOM | 2467 | CD  | GLU | 395 | 86.273 | 71.851 | 97.497  | 1.00 | 25.08 |
| ATOM | 2468 | OE1 | GLU | 395 | 87.250 | 71.342 | 98.094  | 1.00 | 23.12 |
| ATOM | 2469 | OE2 | GLU | 395 | 85.305 | 71.180 | 97.087  | 1.00 | 25.76 |
| ATOM | 2470 | C   | GLU | 395 | 82.772 | 74.976 | 97.629  | 1.00 | 16.80 |
| ATOM | 2471 | O   | GLU | 395 | 82.978 | 76.092 | 97.155  | 1.00 | 17.72 |
| ATOM | 2472 | N   | ALA | 396 | 81.556 | 74.463 | 97.751  | 1.00 | 18.63 |
| ATOM | 2473 | CA  | ALA | 396 | 80.373 | 75.226 | 97.353  | 1.00 | 20.65 |
| ATOM | 2474 | CB  | ALA | 396 | 79.251 | 74.281 | 96.956  | 1.00 | 19.79 |
| ATOM | 2475 | C   | ALA | 396 | 79.926 | 76.131 | 98.496  | 1.00 | 22.38 |
| ATOM | 2476 | O   | ALA | 396 | 80.183 | 75.834 | 99.665  | 1.00 | 23.05 |
| ATOM | 2477 | N   | PRO | 397 | 79.301 | 77.279 | 98.171  | 1.00 | 23.70 |
| ATOM | 2478 | CD  | PRO | 397 | 79.085 | 77.782 | 96.806  | 1.00 | 24.23 |
| ATOM | 2479 | CA  | PRO | 397 | 78.809 | 78.250 | 99.152  | 1.00 | 25.59 |
| ATOM | 2480 | CB  | PRO | 397 | 78.129 | 79.296 | 98.275  | 1.00 | 23.05 |
| ATOM | 2481 | CG  | PRO | 397 | 78.922 | 79.255 | 97.029  | 1.00 | 22.14 |
| ATOM | 2482 | C   | PRO | 397 | 77.811 | 77.637 | 100.133 | 1.00 | 28.01 |
| ATOM | 2483 | O   | PRO | 397 | 77.055 | 76.741 | 99.780  | 1.00 | 28.32 |
| ATOM | 2484 | N   | GLY | 398 | 77.822 | 78.119 | 101.368 | 1.00 | 30.41 |
| ATOM | 2485 | CA  | GLY | 398 | 76.901 | 77.610 | 102.362 | 1.00 | 32.35 |
| ATOM | 2486 | C   | GLY | 398 | 77.536 | 76.719 | 103.406 | 1.00 | 35.07 |
| ATOM | 2487 | O   | GLY | 398 | 78.644 | 76.208 | 103.233 | 1.00 | 34.69 |
| ATOM | 2488 | N   | GLU | 399 | 76.820 | 76.556 | 104.512 | 1.00 | 37.44 |
| ATOM | 2489 | CA  | GLU | 399 | 77.259 | 75.728 | 105.628 | 1.00 | 38.51 |
| ATOM | 2490 | CB  | GLU | 399 | 77.005 | 76.480 | 106.944 | 1.00 | 44.33 |
| ATOM | 2491 | CG  | GLU | 399 | 77.219 | 75.665 | 108.222 | 1.00 | 55.44 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2492 | CD  | GLU | 399 | 75.930 | 75.413 | 109.025 | 1.00 | 65.22 |
| ATOM | 2493 | OE1 | GLU | 399 | 76.015 | 74.743 | 110.082 | 1.00 | 67.57 |
| ATOM | 2494 | OE2 | GLU | 399 | 74.837 | 75.871 | 108.610 | 1.00 | 69.24 |
| ATOM | 2495 | C   | GLU | 399 | 76.488 | 74.407 | 105.603 | 1.00 | 36.40 |
| ATOM | 2496 | O   | GLU | 399 | 75.347 | 74.359 | 105.136 | 1.00 | 36.14 |
| ATOM | 2497 | N   | TYR | 400 | 77.128 | 73.334 | 106.055 | 1.00 | 33.94 |
| ATOM | 2498 | CA  | TYR | 400 | 76.491 | 72.025 | 106.101 | 1.00 | 32.40 |
| ATOM | 2499 | CB  | TYR | 400 | 77.538 | 70.920 | 106.223 | 1.00 | 30.68 |
| ATOM | 2500 | CG  | TYR | 400 | 78.226 | 70.564 | 104.938 | 1.00 | 29.71 |
| ATOM | 2501 | CD1 | TYR | 400 | 77.633 | 69.688 | 104.026 | 1.00 | 28.20 |
| ATOM | 2502 | CE1 | TYR | 400 | 78.274 | 69.344 | 102.845 | 1.00 | 26.95 |
| ATOM | 2503 | CD2 | TYR | 400 | 79.477 | 71.089 | 104.632 | 1.00 | 28.87 |
| ATOM | 2504 | CE2 | TYR | 400 | 80.128 | 70.749 | 103.453 | 1.00 | 27.69 |
| ATOM | 2505 | CZ  | TYR | 400 | 79.523 | 69.882 | 102.565 | 1.00 | 25.06 |
| ATOM | 2506 | OH  | TYR | 400 | 80.169 | 69.554 | 101.403 | 1.00 | 21.76 |
| ATOM | 2507 | C   | TYR | 400 | 75.604 | 71.938 | 107.322 | 1.00 | 32.61 |
| ATOM | 2508 | O   | TYR | 400 | 75.895 | 72.543 | 108.347 | 1.00 | 35.88 |
| ATOM | 2509 | N   | PHE | 401 | 74.542 | 71.160 | 107.235 | 1.00 | 30.97 |
| ATOM | 2510 | CA  | PHE | 401 | 73.670 | 70.985 | 108.376 | 1.00 | 31.87 |
| ATOM | 2511 | CB  | PHE | 401 | 72.514 | 71.999 | 108.356 | 1.00 | 31.10 |
| ATOM | 2512 | CG  | PHE | 401 | 71.644 | 71.914 | 107.133 | 1.00 | 29.98 |
| ATOM | 2513 | CD1 | PHE | 401 | 72.023 | 72.543 | 105.950 | 1.00 | 27.03 |
| ATOM | 2514 | CD2 | PHE | 401 | 70.457 | 71.178 | 107.154 | 1.00 | 25.56 |
| ATOM | 2515 | CE1 | PHE | 401 | 71.238 | 72.438 | 104.806 | 1.00 | 25.34 |
| ATOM | 2516 | CE2 | PHE | 401 | 69.666 | 71.066 | 106.015 | 1.00 | 23.68 |
| ATOM | 2517 | CZ  | PHE | 401 | 70.057 | 71.697 | 104.838 | 1.00 | 25.95 |
| ATOM | 2518 | C   | PHE | 401 | 73.180 | 69.549 | 108.327 | 1.00 | 33.08 |
| ATOM | 2519 | O   | PHE | 401 | 73.597 | 68.779 | 107.465 | 1.00 | 32.13 |
| ATOM | 2520 | N   | PHE | 402 | 72.318 | 69.171 | 109.258 | 1.00 | 35.69 |
| ATOM | 2521 | CA  | PHE | 402 | 71.811 | 67.810 | 109.279 | 1.00 | 37.42 |
| ATOM | 2522 | CB  | PHE | 402 | 72.456 | 67.030 | 110.429 | 1.00 | 35.41 |
| ATOM | 2523 | CG  | PHE | 402 | 73.949 | 66.901 | 110.322 | 1.00 | 32.99 |
| ATOM | 2524 | CD1 | PHE | 402 | 74.525 | 65.726 | 109.847 | 1.00 | 33.35 |
| ATOM | 2525 | CD2 | PHE | 402 | 74.781 | 67.954 | 110.689 | 1.00 | 33.30 |
| ATOM | 2526 | CE1 | PHE | 402 | 75.916 | 65.603 | 109.737 | 1.00 | 31.57 |
| ATOM | 2527 | CE2 | PHE | 402 | 76.167 | 67.844 | 110.584 | 1.00 | 31.22 |
| ATOM | 2528 | CZ  | PHE | 402 | 76.734 | 66.665 | 110.106 | 1.00 | 32.49 |
| ATOM | 2529 | C   | PHE | 402 | 70.291 | 67.770 | 109.418 | 1.00 | 40.49 |
| ATOM | 2530 | O   | PHE | 402 | 69.680 | 68.689 | 109.973 | 1.00 | 41.28 |
| ATOM | 2531 | N   | SER | 403 | 69.689 | 66.726 | 108.862 | 1.00 | 43.51 |
| ATOM | 2532 | CA  | SER | 403 | 68.252 | 66.525 | 108.949 | 1.00 | 47.93 |
| ATOM | 2533 | CB  | SER | 403 | 67.617 | 66.581 | 107.560 | 1.00 | 49.52 |
| ATOM | 2534 | OG  | SER | 403 | 68.245 | 65.660 | 106.683 | 1.00 | 54.86 |
| ATOM | 2535 | C   | SER | 403 | 68.053 | 65.154 | 109.607 | 1.00 | 51.47 |
| ATOM | 2536 | O   | SER | 403 | 68.366 | 64.987 | 110.789 | 1.00 | 53.15 |
| ATOM | 2537 | N   | ASP | 404 | 67.597 | 64.162 | 108.847 | 1.00 | 52.88 |
| ATOM | 2538 | CA  | ASP | 404 | 67.393 | 62.821 | 109.395 | 1.00 | 54.43 |
| ATOM | 2539 | CB  | ASP | 404 | 66.354 | 62.034 | 108.570 | 1.00 | 59.65 |
| ATOM | 2540 | CG  | ASP | 404 | 66.498 | 62.238 | 107.056 | 1.00 | 64.80 |
| ATOM | 2541 | OD1 | ASP | 404 | 65.472 | 62.112 | 106.348 | 1.00 | 66.65 |
| ATOM | 2542 | OD2 | ASP | 404 | 67.617 | 62.520 | 106.569 | 1.00 | 67.01 |
| ATOM | 2543 | C   | ASP | 404 | 68.727 | 62.080 | 109.468 | 1.00 | 53.52 |
| ATOM | 2544 | O   | ASP | 404 | 68.899 | 61.003 | 108.893 | 1.00 | 54.08 |
| ATOM | 2545 | N   | GLY | 405 | 69.673 | 62.674 | 110.186 | 1.00 | 52.57 |
| ATOM | 2546 | CA  | GLY | 405 | 70.989 | 62.080 | 110.314 | 1.00 | 51.71 |
| ATOM | 2547 | C   | GLY | 405 | 71.745 | 62.165 | 109.004 | 1.00 | 50.71 |
| ATOM | 2548 | O   | GLY | 405 | 72.761 | 61.494 | 108.817 | 1.00 | 51.94 |
| ATOM | 2549 | N   | ILE | 406 | 71.254 | 63.006 | 108.101 | 1.00 | 49.32 |

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FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2550 | CA  | ILE | 406 | 71.873 | 63.185 | 106.797 | 1.00 | 46.50 |
| ATOM | 2551 | CB  | ILE | 406 | 70.868 | 62.860 | 105.670 | 1.00 | 45.63 |
| ATOM | 2552 | CG2 | ILE | 406 | 71.409 | 63.303 | 104.321 | 1.00 | 45.90 |
| ATOM | 2553 | CG1 | ILE | 406 | 70.585 | 61.353 | 105.677 | 1.00 | 47.65 |
| ATOM | 2554 | CD1 | ILE | 406 | 69.620 | 60.887 | 104.620 | 1.00 | 51.01 |
| ATOM | 2555 | C   | ILE | 406 | 72.443 | 64.592 | 106.648 | 1.00 | 44.89 |
| ATOM | 2556 | O   | ILE | 406 | 71.744 | 65.588 | 106.886 | 1.00 | 45.23 |
| ATOM | 2557 | N   | ARG | 407 | 73.727 | 64.662 | 106.306 | 1.00 | 42.16 |
| ATOM | 2558 | CA  | ARG | 407 | 74.403 | 65.939 | 106.137 | 1.00 | 39.23 |
| ATOM | 2559 | CB  | ARG | 407 | 75.918 | 65.756 | 106.126 | 1.00 | 38.21 |
| ATOM | 2560 | CG  | ARG | 407 | 76.668 | 67.017 | 106.504 | 1.00 | 36.68 |
| ATOM | 2561 | CD  | ARG | 407 | 78.142 | 66.747 | 106.691 | 1.00 | 38.88 |
| ATOM | 2562 | NE  | ARG | 407 | 78.743 | 67.742 | 107.571 | 1.00 | 41.10 |
| ATOM | 2563 | CZ  | ARG | 407 | 79.902 | 68.347 | 107.343 | 1.00 | 40.51 |
| ATOM | 2564 | NH1 | ARG | 407 | 80.604 | 68.063 | 106.255 | 1.00 | 36.09 |
| ATOM | 2565 | NH2 | ARG | 407 | 80.346 | 69.258 | 108.198 | 1.00 | 40.72 |
| ATOM | 2566 | C   | ARG | 407 | 73.944 | 66.546 | 104.831 | 1.00 | 37.51 |
| ATOM | 2567 | O   | ARG | 407 | 73.902 | 65.867 | 103.805 | 1.00 | 39.48 |
| ATOM | 2568 | N   | LEU | 408 | 73.601 | 67.824 | 104.868 | 1.00 | 34.38 |
| ATOM | 2569 | CA  | LEU | 408 | 73.115 | 68.504 | 103.683 | 1.00 | 31.16 |
| ATOM | 2570 | CB  | LEU | 408 | 71.588 | 68.562 | 103.724 | 1.00 | 24.97 |
| ATOM | 2571 | CG  | LEU | 408 | 70.844 | 67.249 | 103.927 | 1.00 | 20.15 |
| ATOM | 2572 | CD1 | LEU | 408 | 69.476 | 67.526 | 104.499 | 1.00 | 19.69 |
| ATOM | 2573 | CD2 | LEU | 408 | 70.784 | 66.473 | 102.631 | 1.00 | 14.81 |
| ATOM | 2574 | C   | LEU | 408 | 73.656 | 69.921 | 103.581 | 1.00 | 31.84 |
| ATOM | 2575 | O   | LEU | 408 | 74.160 | 70.493 | 104.551 | 1.00 | 33.47 |
| ATOM | 2576 | N   | LYS | 409 | 73.548 | 70.470 | 102.381 | 1.00 | 30.46 |
| ATOM | 2577 | CA  | LYS | 409 | 73.967 | 71.827 | 102.091 | 1.00 | 27.79 |
| ATOM | 2578 | CR  | LYS | 409 | 75.332 | 71.834 | 101.402 | 1.00 | 27.10 |
| ATOM | 2579 | CG  | LYS | 409 | 75.988 | 73.200 | 101.349 | 1.00 | 26.08 |
| ATOM | 2580 | CD  | LYS | 409 | 77.168 | 73.220 | 100.398 | 1.00 | 26.04 |
| ATOM | 2581 | CE  | LYS | 409 | 78.425 | 72.632 | 100.998 | 1.00 | 25.41 |
| ATOM | 2582 | NZ  | LYS | 409 | 79.076 | 73.542 | 101.965 | 1.00 | 24.68 |
| ATOM | 2583 | C   | LYS | 409 | 72.878 | 72.320 | 101.142 | 1.00 | 26.84 |
| ATOM | 2584 | O   | LYS | 409 | 72.376 | 71.562 | 100.311 | 1.00 | 26.63 |
| ATOM | 2585 | N   | LYS | 410 | 72.495 | 73.577 | 101.285 | 1.00 | 26.58 |
| ATOM | 2586 | CA  | LYS | 410 | 71.452 | 74.169 | 100.468 | 1.00 | 27.15 |
| ATOM | 2587 | CB  | LYS | 410 | 71.132 | 75.568 | 100.993 | 1.00 | 31.97 |
| ATOM | 2588 | CG  | LYS | 410 | 70.054 | 75.605 | 102.062 | 1.00 | 40.07 |
| ATOM | 2589 | CD  | LYS | 410 | 68.680 | 75.378 | 101.442 | 1.00 | 46.67 |
| ATOM | 2590 | CE  | LYS | 410 | 68.389 | 76.403 | 100.339 | 1.00 | 47.01 |
| ATOM | 2591 | NZ  | LYS | 410 | 67.072 | 76.159 | 99.700  | 1.00 | 43.19 |
| ATOM | 2592 | C   | LYS | 410 | 71.758 | 74.260 | 98.980  | 1.00 | 25.29 |
| ATOM | 2593 | O   | LYS | 410 | 72.895 | 74.479 | 98.576  | 1.00 | 25.69 |
| ATOM | 2594 | N   | TYR | 411 | 70.725 | 74.071 | 98.174  | 1.00 | 22.53 |
| ATOM | 2595 | CA  | TYR | 411 | 70.830 | 74.192 | 96.735  | 1.00 | 19.58 |
| ATOM | 2596 | CB  | TYR | 411 | 71.035 | 72.840 | 96.051  | 1.00 | 16.64 |
| ATOM | 2597 | CG  | TYR | 411 | 71.132 | 72.979 | 94.546  | 1.00 | 18.10 |
| ATOM | 2598 | CD1 | TYR | 411 | 71.895 | 74.000 | 93.974  | 1.00 | 18.77 |
| ATOM | 2599 | CE1 | TYR | 411 | 71.929 | 74.196 | 92.605  | 1.00 | 19.48 |
| ATOM | 2600 | CD2 | TYR | 411 | 70.409 | 72.145 | 93.693  | 1.00 | 17.87 |
| ATOM | 2601 | CE2 | TYR | 411 | 70.439 | 72.334 | 92.310  | 1.00 | 17.72 |
| ATOM | 2602 | CZ  | TYR | 411 | 71.199 | 73.367 | 91.774  | 1.00 | 19.31 |
| ATOM | 2603 | OH  | TYR | 411 | 71.210 | 73.599 | 90.412  | 1.00 | 22.34 |
| ATOM | 2604 | C   | TYR | 411 | 69.510 | 74.820 | 96.295  | 1.00 | 20.78 |
| ATOM | 2605 | O   | TYR | 411 | 68.432 | 74.278 | 96.570  | 1.00 | 20.50 |
| ATOM | 2606 | N   | ARG | 412 | 69.582 | 75.968 | 95.631  | 1.00 | 19.85 |
| ATOM | 2607 | CA  | ARG | 412 | 68.368 | 76.641 | 95.199  | 1.00 | 18.82 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2608 | CB  | ARG | 412 | 67.992 | 77.750 | 96.187  | 1.00 | 16.10 |
| ATOM | 2609 | CG  | ARG | 412 | 68.919 | 78.944 | 96.139  | 1.00 | 13.54 |
| ATOM | 2610 | CD  | ARG | 412 | 68.454 | 80.049 | 97.034  | 1.00 | 10.34 |
| ATOM | 2611 | NE  | ARG | 412 | 69.325 | 81.207 | 96.904  | 1.00 | 17.42 |
| ATOM | 2612 | CZ  | ARG | 412 | 69.384 | 82.205 | 97.782  | 1.00 | 21.02 |
| ATOM | 2613 | NH1 | ARG | 412 | 68.621 | 82.193 | 98.864  | 1.00 | 22.12 |
| ATOM | 2614 | NH2 | ARG | 412 | 70.217 | 83.217 | 97.586  | 1.00 | 23.60 |
| ATOM | 2615 | C   | ARG | 412 | 68.464 | 77.235 | 93.808  | 1.00 | 20.49 |
| ATOM | 2616 | O   | ARG | 412 | 69.510 | 77.762 | 93.401  | 1.00 | 19.42 |
| ATOM | 2617 | N   | GLY | 413 | 67.348 | 77.168 | 93.092  | 1.00 | 22.45 |
| ATOM | 2618 | CA  | GLY | 413 | 67.295 | 77.725 | 91.759  | 1.00 | 22.08 |
| ATOM | 2619 | C   | GLY | 413 | 67.358 | 79.233 | 91.846  | 1.00 | 20.93 |
| ATOM | 2620 | O   | GLY | 413 | 66.791 | 79.831 | 92.761  | 1.00 | 19.19 |
| ATOM | 2621 | N   | MET | 414 | 68.049 | 79.845 | 90.893  | 1.00 | 21.29 |
| ATOM | 2622 | CA  | MET | 414 | 68.197 | 81.292 | 90.847  | 1.00 | 21.49 |
| ATOM | 2623 | CB  | MET | 414 | 69.265 | 81.681 | 89.824  | 1.00 | 23.96 |
| ATOM | 2624 | CG  | MET | 414 | 70.672 | 81.250 | 90.224  | 1.00 | 21.70 |
| ATOM | 2625 | SD  | MET | 414 | 71.103 | 81.734 | 91.919  | 1.00 | 18.54 |
| ATOM | 2626 | CE  | MET | 414 | 71.695 | 83.398 | 91.646  | 1.00 | 23.85 |
| ATOM | 2627 | C   | MET | 414 | 66.888 | 82.025 | 90.567  | 1.00 | 20.64 |
| ATOM | 2628 | O   | MET | 414 | 66.822 | 83.254 | 90.648  | 1.00 | 20.74 |
| ATOM | 2629 | N   | GLY | 415 | 65.854 | 81.267 | 90.233  | 1.00 | 20.53 |
| ATOM | 2630 | CA  | GLY | 415 | 64.558 | 81.851 | 89.972  | 1.00 | 19.68 |
| ATOM | 2631 | C   | GLY | 415 | 63.640 | 81.592 | 91.147  | 1.00 | 21.08 |
| ATOM | 2632 | O   | GLY | 415 | 62.425 | 81.726 | 91.021  | 1.00 | 23.65 |
| ATOM | 2633 | N   | SER | 416 | 64.197 | 81.142 | 92.266  | 1.00 | 20.91 |
| ATOM | 2634 | CA  | SER | 416 | 63.393 | 80.886 | 93.455  | 1.00 | 22.71 |
| ATOM | 2635 | CB  | SER | 416 | 64.144 | 79.996 | 94.451  | 1.00 | 22.91 |
| ATOM | 2636 | OG  | SER | 416 | 65.344 | 80.599 | 94.910  | 1.00 | 20.96 |
| ATOM | 2637 | C   | SER | 416 | 63.105 | 82.236 | 94.087  | 1.00 | 24.99 |
| ATOM | 2638 | O   | SER | 416 | 63.870 | 83.181 | 93.890  | 1.00 | 27.08 |
| ATOM | 2639 | N   | LEU | 417 | 62.019 | 82.337 | 94.846  | 1.00 | 26.49 |
| ATOM | 2640 | CA  | LEU | 417 | 61.679 | 83.601 | 95.485  | 1.00 | 29.42 |
| ATOM | 2641 | CB  | LEU | 417 | 60.362 | 83.497 | 96.255  | 1.00 | 31.14 |
| ATOM | 2642 | CG  | LEU | 417 | 59.054 | 83.276 | 95.486  | 1.00 | 30.31 |
| ATOM | 2643 | CD1 | LEU | 417 | 57.907 | 83.354 | 96.474  | 1.00 | 30.36 |
| ATOM | 2644 | CD2 | LEU | 417 | 58.862 | 84.302 | 94.378  | 1.00 | 25.63 |
| ATOM | 2645 | C   | LEU | 417 | 62.795 | 84.055 | 96.420  | 1.00 | 32.03 |
| ATOM | 2646 | O   | LEU | 417 | 63.061 | 85.249 | 96.532  | 1.00 | 33.75 |
| ATOM | 2647 | N   | ASP | 418 | 63.445 | 83.095 | 97.081  | 1.00 | 35.21 |
| ATOM | 2648 | CA  | ASP | 418 | 64.550 | 83.378 | 98.005  | 1.00 | 35.94 |
| ATOM | 2649 | CB  | ASP | 418 | 64.942 | 82.121 | 98.797  | 1.00 | 35.59 |
| ATOM | 2650 | CG  | ASP | 418 | 63.988 | 81.821 | 99.942  | 1.00 | 39.46 |
| ATOM | 2651 | OD1 | ASP | 418 | 63.295 | 82.749 | 100.423 | 1.00 | 40.20 |
| ATOM | 2652 | OD2 | ASP | 418 | 63.941 | 80.651 | 100.374 | 1.00 | 41.70 |
| ATOM | 2653 | C   | ASP | 418 | 65.777 | 83.902 | 97.275  | 1.00 | 36.50 |
| ATOM | 2654 | O   | ASP | 418 | 66.407 | 84.860 | 97.716  | 1.00 | 37.43 |
| ATOM | 2655 | N   | ALA | 419 | 66.147 | 83.233 | 96.189  | 1.00 | 36.59 |
| ATOM | 2656 | CA  | ALA | 419 | 67.301 | 83.646 | 95.411  | 1.00 | 37.48 |
| ATOM | 2657 | CB  | ALA | 419 | 67.567 | 82.660 | 94.300  | 1.00 | 36.03 |
| ATOM | 2658 | C   | ALA | 419 | 67.021 | 85.024 | 94.841  | 1.00 | 39.11 |
| ATOM | 2659 | O   | ALA | 419 | 67.914 | 85.869 | 94.774  | 1.00 | 40.78 |
| ATOM | 2660 | N   | MET | 420 | 65.770 | 85.245 | 94.446  | 1.00 | 39.62 |
| ATOM | 2661 | CA  | MET | 420 | 65.348 | 86.521 | 93.884  | 1.00 | 40.26 |
| ATOM | 2662 | CB  | MET | 420 | 64.039 | 86.368 | 93.096  | 1.00 | 40.92 |
| ATOM | 2663 | CG  | MET | 420 | 64.124 | 85.453 | 91.879  | 1.00 | 38.85 |
| ATOM | 2664 | SD  | MET | 420 | 62.752 | 85.698 | 90.733  | 1.00 | 35.95 |
| ATOM | 2665 | CE  | MET | 420 | 61.390 | 84.999 | 91.678  | 1.00 | 32.77 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2666 | C   | MET | 420 | 65.163 | 87.549 | 94.991 | 1.00 | 40.67 |
| ATOM | 2667 | O   | MET | 420 | 65.352 | 88.741 | 94.681 | 1.00 | 41.51 |
| ATOM | 2668 | CB  | ILE | 437 | 53.259 | 89.508 | 90.596 | 1.00 | 46.60 |
| ATOM | 2669 | CG2 | ILE | 437 | 53.123 | 88.263 | 91.473 | 1.00 | 42.38 |
| ATOM | 2670 | CG1 | ILE | 437 | 52.015 | 90.393 | 90.752 | 1.00 | 48.50 |
| ATOM | 2671 | CD1 | ILE | 437 | 51.671 | 91.225 | 89.513 | 1.00 | 48.60 |
| ATOM | 2672 | C   | ILE | 437 | 55.751 | 89.463 | 90.476 | 1.00 | 46.43 |
| ATOM | 2673 | O   | ILE | 437 | 56.179 | 89.615 | 89.324 | 1.00 | 47.38 |
| ATOM | 2674 | N   | ILE | 437 | 54.637 | 91.629 | 90.302 | 1.00 | 47.00 |
| ATOM | 2675 | CA  | ILE | 437 | 54.566 | 90.290 | 90.965 | 1.00 | 47.20 |
| ATOM | 2676 | N   | LYS | 438 | 56.291 | 88.622 | 91.355 | 1.00 | 43.78 |
| ATOM | 2677 | CA  | LYS | 438 | 57.413 | 87.764 | 91.001 | 1.00 | 40.48 |
| ATOM | 2678 | CB  | LYS | 438 | 58.472 | 87.761 | 92.100 | 1.00 | 43.36 |
| ATOM | 2679 | CG  | LYS | 438 | 59.340 | 89.005 | 92.099 | 1.00 | 52.37 |
| ATOM | 2680 | CD  | LYS | 438 | 60.428 | 88.957 | 93.164 | 1.00 | 57.07 |
| ATOM | 2681 | CE  | LYS | 438 | 61.260 | 90.234 | 93.136 | 1.00 | 57.16 |
| ATOM | 2682 | NZ  | LYS | 438 | 62.246 | 90.282 | 94.245 | 1.00 | 58.75 |
| ATOM | 2683 | C   | LYS | 438 | 56.919 | 86.350 | 90.749 | 1.00 | 37.61 |
| ATOM | 2684 | O   | LYS | 438 | 56.197 | 85.778 | 91.564 | 1.00 | 37.45 |
| ATOM | 2685 | N   | VAL | 439 | 57.249 | 85.835 | 89.572 | 1.00 | 34.22 |
| ATOM | 2686 | CA  | VAL | 439 | 56.871 | 84.489 | 89.175 | 1.00 | 29.77 |
| ATOM | 2687 | CB  | VAL | 439 | 56.519 | 84.430 | 87.670 | 1.00 | 25.38 |
| ATOM | 2688 | CG1 | VAL | 439 | 56.312 | 82.994 | 87.224 | 1.00 | 24.88 |
| ATOM | 2689 | CG2 | VAL | 439 | 55.279 | 85.246 | 87.396 | 1.00 | 22.94 |
| ATOM | 2690 | C   | VAL | 439 | 58.098 | 83.637 | 89.436 | 1.00 | 29.52 |
| ATOM | 2691 | O   | VAL | 439 | 59.152 | 83.867 | 88.836 | 1.00 | 30.63 |
| ATOM | 2692 | N   | ALA | 440 | 57.991 | 82.723 | 90.392 | 1.00 | 28.23 |
| ATOM | 2693 | CA  | ALA | 440 | 59.104 | 81.843 | 90.720 | 1.00 | 26.56 |
| ATOM | 2694 | CB  | ALA | 440 | 58.859 | 81.151 | 92.037 | 1.00 | 23.10 |
| ATOM | 2695 | C   | ALA | 440 | 59.277 | 80.818 | 89.606 | 1.00 | 26.95 |
| ATOM | 2696 | O   | ALA | 440 | 58.298 | 80.297 | 89.072 | 1.00 | 28.49 |
| ATOM | 2697 | N   | GLN | 441 | 60.524 | 80.584 | 89.212 | 1.00 | 26.65 |
| ATOM | 2698 | CA  | GLN | 441 | 60.841 | 79.625 | 88.163 | 1.00 | 23.30 |
| ATOM | 2699 | CB  | GLN | 441 | 61.463 | 80.328 | 86.967 | 1.00 | 22.34 |
| ATOM | 2700 | CG  | GLN | 441 | 60.483 | 81.223 | 86.245 | 1.00 | 26.34 |
| ATOM | 2701 | CD  | GLN | 441 | 61.126 | 81.994 | 85.126 | 1.00 | 30.83 |
| ATOM | 2702 | OE1 | GLN | 441 | 61.199 | 83.226 | 85.164 | 1.00 | 32.45 |
| ATOM | 2703 | NE2 | GLN | 441 | 61.608 | 81.277 | 84.119 | 1.00 | 32.37 |
| ATOM | 2704 | C   | GLN | 441 | 61.787 | 78.582 | 88.700 | 1.00 | 22.70 |
| ATOM | 2705 | O   | GLN | 441 | 62.100 | 77.609 | 88.017 | 1.00 | 24.78 |
| ATOM | 2706 | N   | GLY | 442 | 62.192 | 78.763 | 89.949 | 1.00 | 21.19 |
| ATOM | 2707 | CA  | GLY | 442 | 63.092 | 77.828 | 90.584 | 1.00 | 21.43 |
| ATOM | 2708 | C   | GLY | 442 | 62.534 | 77.485 | 91.945 | 1.00 | 21.81 |
| ATOM | 2709 | O   | GLY | 442 | 61.635 | 78.168 | 92.436 | 1.00 | 22.56 |
| ATOM | 2710 | N   | VAL | 443 | 63.117 | 76.471 | 92.574 | 1.00 | 21.86 |
| ATOM | 2711 | CA  | VAL | 443 | 62.699 | 75.985 | 93.886 | 1.00 | 20.15 |
| ATOM | 2712 | CB  | VAL | 443 | 62.124 | 74.542 | 93.720 | 1.00 | 19.51 |
| ATOM | 2713 | CG1 | VAL | 443 | 62.997 | 73.490 | 94.406 | 1.00 | 18.43 |
| ATOM | 2714 | CG2 | VAL | 443 | 60.692 | 74.487 | 94.176 | 1.00 | 20.94 |
| ATOM | 2715 | C   | VAL | 443 | 63.908 | 76.010 | 94.839 | 1.00 | 20.65 |
| ATOM | 2716 | O   | VAL | 443 | 65.054 | 76.084 | 94.381 | 1.00 | 20.98 |
| ATOM | 2717 | N   | SER | 444 | 63.657 | 75.985 | 96.149 | 1.00 | 21.18 |
| ATOM | 2718 | CA  | SER | 444 | 64.733 | 75.988 | 97.149 | 1.00 | 21.80 |
| ATOM | 2719 | CB  | SER | 444 | 64.582 | 77.171 | 98.108 | 1.00 | 24.85 |
| ATOM | 2720 | OG  | SER | 444 | 64.906 | 78.399 | 97.480 | 1.00 | 33.77 |
| ATOM | 2721 | C   | SER | 444 | 64.827 | 74.688 | 97.960 | 1.00 | 22.20 |
| ATOM | 2722 | O   | SER | 444 | 63.955 | 74.394 | 98.791 | 1.00 | 23.12 |
| ATOM | 2723 | N   | GLY | 445 | 65.917 | 73.948 | 97.777 | 1.00 | 21.40 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2724 | CA  | GLY | 445 | 66.068 | 72.700 | 98.495  | 1.00 | 22.02 |
| ATOM | 2725 | C   | GLY | 445 | 67.439 | 72.436 | 99.076  | 1.00 | 23.53 |
| ATOM | 2726 | O   | GLY | 445 | 68.217 | 73.362 | 99.316  | 1.00 | 25.01 |
| ATOM | 2727 | N   | ALA | 446 | 67.729 | 71.164 | 99.319  | 1.00 | 22.46 |
| ATOM | 2728 | CA  | ALA | 446 | 69.004 | 70.768 | 99.890  | 1.00 | 21.42 |
| ATOM | 2729 | CB  | ALA | 446 | 68.890 | 70.614 | 101.396 | 1.00 | 19.79 |
| ATOM | 2730 | C   | ALA | 446 | 69.422 | 69.459 | 99.277  | 1.00 | 22.96 |
| ATOM | 2731 | O   | ALA | 446 | 68.576 | 68.627 | 98.946  | 1.00 | 24.40 |
| ATOM | 2732 | N   | VAL | 447 | 70.731 | 69.287 | 99.129  | 1.00 | 24.30 |
| ATOM | 2733 | CA  | VAL | 447 | 71.326 | 68.080 | 98.572  | 1.00 | 23.81 |
| ATOM | 2734 | CB  | VAL | 447 | 72.068 | 68.389 | 97.260  | 1.00 | 22.59 |
| ATOM | 2735 | CG1 | VAL | 447 | 71.078 | 68.801 | 96.195  | 1.00 | 23.88 |
| ATOM | 2736 | CG2 | VAL | 447 | 73.048 | 69.515 | 97.467  | 1.00 | 28.09 |
| ATOM | 2737 | C   | VAL | 447 | 72.284 | 67.467 | 99.607  | 1.00 | 25.54 |
| ATOM | 2738 | O   | VAL | 447 | 72.765 | 68.155 | 100.510 | 1.00 | 26.03 |
| ATOM | 2739 | N   | GLN | 448 | 72.530 | 66.168 | 99.491  | 1.00 | 26.62 |
| ATOM | 2740 | CA  | GLN | 448 | 73.401 | 65.460 | 100.420 | 1.00 | 27.39 |
| ATOM | 2741 | CB  | GLN | 448 | 73.033 | 63.973 | 100.424 | 1.00 | 30.61 |
| ATOM | 2742 | CG  | GLN | 448 | 73.722 | 63.113 | 101.477 | 1.00 | 33.45 |
| ATOM | 2743 | CD  | GLN | 448 | 73.330 | 61.636 | 101.390 | 1.00 | 36.95 |
| ATOM | 2744 | OE1 | GLN | 448 | 73.820 | 60.811 | 102.160 | 1.00 | 40.13 |
| ATOM | 2745 | NE2 | GLN | 448 | 72.443 | 61.300 | 100.454 | 1.00 | 37.67 |
| ATOM | 2746 | C   | GLN | 448 | 74.877 | 65.654 | 100.068 | 1.00 | 28.24 |
| ATOM | 2747 | O   | GLN | 448 | 75.249 | 65.660 | 98.896  | 1.00 | 30.00 |
| ATOM | 2748 | N   | ASP | 449 | 75.694 | 65.816 | 101.106 | 1.00 | 29.14 |
| ATOM | 2749 | CA  | ASP | 449 | 77.142 | 66.029 | 101.025 | 1.00 | 26.21 |
| ATOM | 2750 | CB  | ASP | 449 | 77.724 | 65.825 | 102.434 | 1.00 | 28.70 |
| ATOM | 2751 | CG  | ASP | 449 | 79.212 | 66.116 | 102.524 | 1.00 | 33.19 |
| ATOM | 2752 | OD1 | ASP | 449 | 79.789 | 66.694 | 101.582 | 1.00 | 35.84 |
| ATOM | 2753 | OD2 | ASP | 449 | 79.811 | 65.771 | 103.566 | 1.00 | 34.41 |
| ATOM | 2754 | C   | ASP | 449 | 77.842 | 65.112 | 100.022 | 1.00 | 23.36 |
| ATOM | 2755 | O   | ASP | 449 | 77.731 | 63.895 | 100.114 | 1.00 | 23.48 |
| ATOM | 2756 | N   | LYS | 450 | 78.582 | 65.708 | 99.087  | 1.00 | 23.13 |
| ATOM | 2757 | CA  | LYS | 450 | 79.319 | 64.962 | 98.056  | 1.00 | 23.09 |
| ATOM | 2758 | CB  | LYS | 450 | 79.048 | 65.539 | 96.665  | 1.00 | 24.74 |
| ATOM | 2759 | CG  | LYS | 450 | 77.600 | 65.522 | 96.251  | 1.00 | 30.34 |
| ATOM | 2760 | CD  | LYS | 450 | 77.445 | 65.993 | 94.816  | 1.00 | 34.49 |
| ATOM | 2761 | CE  | LYS | 450 | 75.982 | 66.200 | 94.487  | 1.00 | 38.17 |
| ATOM | 2762 | NZ  | LYS | 450 | 75.383 | 67.270 | 95.338  | 1.00 | 42.96 |
| ATOM | 2763 | C   | LYS | 450 | 80.833 | 64.953 | 98.281  | 1.00 | 23.02 |
| ATOM | 2764 | O   | LYS | 450 | 81.582 | 64.347 | 97.507  | 1.00 | 21.57 |
| ATOM | 2765 | N   | GLY | 451 | 81.283 | 65.643 | 99.321  | 1.00 | 22.90 |
| ATOM | 2766 | CA  | GLY | 451 | 82.701 | 65.694 | 99.611  | 1.00 | 23.16 |
| ATOM | 2767 | C   | GLY | 451 | 83.381 | 66.831 | 98.874  | 1.00 | 23.95 |
| ATOM | 2768 | O   | GLY | 451 | 82.729 | 67.801 | 98.485  | 1.00 | 24.66 |
| ATOM | 2769 | N   | SER | 452 | 84.689 | 66.704 | 98.663  | 1.00 | 22.79 |
| ATOM | 2770 | CA  | SER | 452 | 85.464 | 67.735 | 97.990  | 1.00 | 19.59 |
| ATOM | 2771 | CB  | SER | 452 | 86.909 | 67.718 | 98.502  | 1.00 | 19.37 |
| ATOM | 2772 | OG  | SER | 452 | 87.726 | 68.650 | 97.808  | 1.00 | 19.18 |
| ATOM | 2773 | C   | SER | 452 | 85.463 | 67.616 | 96.482  | 1.00 | 17.85 |
| ATOM | 2774 | O   | SER | 452 | 85.449 | 66.514 | 95.936  | 1.00 | 19.84 |
| ATOM | 2775 | N   | ILE | 453 | 85.547 | 68.766 | 95.820  | 1.00 | 16.24 |
| ATOM | 2776 | CA  | ILE | 453 | 85.604 | 68.843 | 94.369  | 1.00 | 14.58 |
| ATOM | 2777 | CB  | ILE | 453 | 85.722 | 70.307 | 93.884  | 1.00 | 12.83 |
| ATOM | 2778 | CG2 | ILE | 453 | 86.387 | 70.376 | 92.525  | 1.00 | 10.62 |
| ATOM | 2779 | CG1 | ILE | 453 | 84.349 | 70.958 | 93.807  | 1.00 | 14.75 |
| ATOM | 2780 | CD1 | ILE | 453 | 83.437 | 70.321 | 92.791  | 1.00 | 14.86 |
| ATOM | 2781 | C   | ILE | 453 | 86.880 | 68.118 | 93.990  | 1.00 | 16.06 |



FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2782 | O   | ILE | 453 | 86.919 | 67.393 | 93.005 | 1.00 | 17.00 |
| ATOM | 2783 | N   | HIS | 454 | 87.900 | 68.257 | 94.831 | 1.00 | 17.66 |
| ATOM | 2784 | CA  | HIS | 454 | 89.191 | 67.626 | 94.575 | 1.00 | 20.84 |
| ATOM | 2785 | CB  | HIS | 454 | 90.263 | 68.161 | 95.534 | 1.00 | 21.96 |
| ATOM | 2786 | CG  | HIS | 454 | 90.627 | 69.594 | 95.290 | 1.00 | 25.98 |
| ATOM | 2787 | CD2 | HIS | 454 | 90.299 | 70.725 | 95.961 | 1.00 | 27.87 |
| ATOM | 2788 | ND1 | HIS | 454 | 91.410 | 69.996 | 94.228 | 1.00 | 28.38 |
| ATOM | 2789 | CE1 | HIS | 454 | 91.551 | 71.312 | 94.254 | 1.00 | 27.52 |
| ATOM | 2790 | NE2 | HIS | 454 | 90.885 | 71.777 | 95.297 | 1.00 | 28.90 |
| ATOM | 2791 | C   | HIS | 454 | 89.160 | 66.096 | 94.564 | 1.00 | 20.36 |
| ATOM | 2792 | O   | HIS | 454 | 90.147 | 65.449 | 94.206 | 1.00 | 19.89 |
| ATOM | 2793 | N   | LYS | 455 | 88.032 | 65.516 | 94.950 | 1.00 | 19.40 |
| ATOM | 2794 | CA  | LYS | 455 | 87.909 | 64.070 | 94.926 | 1.00 | 21.55 |
| ATOM | 2795 | CB  | LYS | 455 | 87.551 | 63.520 | 96.308 | 1.00 | 23.22 |
| ATOM | 2796 | CG  | LYS | 455 | 88.653 | 63.668 | 97.367 | 1.00 | 29.03 |
| ATOM | 2797 | CD  | LYS | 455 | 89.945 | 62.933 | 96.994 | 1.00 | 37.13 |
| ATOM | 2798 | CE  | LYS | 455 | 89.757 | 61.421 | 96.873 | 1.00 | 45.38 |
| ATOM | 2799 | NZ  | LYS | 455 | 89.383 | 60.783 | 98.171 | 1.00 | 51.78 |
| ATOM | 2800 | C   | LYS | 455 | 86.819 | 63.728 | 93.920 | 1.00 | 22.09 |
| ATOM | 2801 | O   | LYS | 455 | 86.992 | 62.862 | 93.051 | 1.00 | 21.63 |
| ATOM | 2802 | N   | PHE | 456 | 85.733 | 64.489 | 93.980 | 1.00 | 21.70 |
| ATOM | 2803 | CA  | PHE | 456 | 84.599 | 64.272 | 93.101 | 1.00 | 20.89 |
| ATOM | 2804 | CB  | PHE | 456 | 83.416 | 65.142 | 93.523 | 1.00 | 18.96 |
| ATOM | 2805 | CG  | PHE | 456 | 82.130 | 64.771 | 92.858 | 1.00 | 16.22 |
| ATOM | 2806 | CD1 | PHE | 456 | 81.401 | 63.671 | 93.296 | 1.00 | 18.25 |
| ATOM | 2807 | CD2 | PHE | 456 | 81.641 | 65.521 | 91.796 | 1.00 | 15.63 |
| ATOM | 2808 | CE1 | PHE | 456 | 80.197 | 63.319 | 92.684 | 1.00 | 19.07 |
| ATOM | 2809 | CE2 | PHE | 456 | 80.446 | 65.184 | 91.177 | 1.00 | 17.34 |
| ATOM | 2810 | CZ  | PHE | 456 | 79.719 | 64.078 | 91.622 | 1.00 | 20.36 |
| ATOM | 2811 | C   | PHE | 456 | 84.918 | 64.487 | 91.632 | 1.00 | 19.73 |
| ATOM | 2812 | O   | PHE | 456 | 84.580 | 63.636 | 90.805 | 1.00 | 22.69 |
| ATOM | 2813 | N   | VAL | 457 | 85.563 | 65.601 | 91.296 | 1.00 | 17.27 |
| ATOM | 2814 | CA  | VAL | 457 | 85.891 | 65.868 | 89.899 | 1.00 | 17.66 |
| ATOM | 2815 | CB  | VAL | 457 | 86.424 | 67.307 | 89.664 | 1.00 | 18.94 |
| ATOM | 2816 | CG1 | VAL | 457 | 86.985 | 67.457 | 88.240 | 1.00 | 16.68 |
| ATOM | 2817 | CG2 | VAL | 457 | 85.281 | 68.295 | 89.853 | 1.00 | 16.75 |
| ATOM | 2818 | C   | VAL | 457 | 86.799 | 64.800 | 89.298 | 1.00 | 16.95 |
| ATOM | 2819 | O   | VAL | 457 | 86.588 | 64.383 | 88.158 | 1.00 | 18.92 |
| ATOM | 2820 | N   | PRO | 458 | 87.833 | 64.358 | 90.035 | 1.00 | 16.13 |
| ATOM | 2821 | CD  | PRO | 458 | 88.457 | 64.985 | 91.214 | 1.00 | 15.29 |
| ATOM | 2822 | CA  | PRO | 458 | 88.710 | 63.313 | 89.489 | 1.00 | 15.15 |
| ATOM | 2823 | CB  | PRO | 458 | 89.669 | 63.058 | 90.638 | 1.00 | 12.23 |
| ATOM | 2824 | CG  | PRO | 458 | 89.866 | 64.440 | 91.171 | 1.00 | 13.07 |
| ATOM | 2825 | C   | PRO | 458 | 87.881 | 62.074 | 89.176 | 1.00 | 15.35 |
| ATOM | 2826 | O   | PRO | 458 | 88.106 | 61.392 | 88.168 | 1.00 | 15.34 |
| ATOM | 2827 | N   | TYR | 459 | 86.901 | 61.809 | 90.034 | 1.00 | 17.57 |
| ATOM | 2828 | CA  | TYR | 459 | 86.008 | 60.675 | 89.856 | 1.00 | 18.14 |
| ATOM | 2829 | CB  | TYR | 459 | 85.077 | 60.521 | 91.059 | 1.00 | 17.11 |
| ATOM | 2830 | CG  | TYR | 459 | 83.808 | 59.775 | 90.725 | 1.00 | 21.11 |
| ATOM | 2831 | CD1 | TYR | 459 | 83.826 | 58.407 | 90.420 | 1.00 | 18.93 |
| ATOM | 2832 | CE1 | TYR | 459 | 82.671 | 57.751 | 90.004 | 1.00 | 14.76 |
| ATOM | 2833 | CD2 | TYR | 459 | 82.597 | 60.457 | 90.625 | 1.00 | 20.85 |
| ATOM | 2834 | CE2 | TYR | 459 | 81.446 | 59.815 | 90.213 | 1.00 | 15.55 |
| ATOM | 2835 | CZ  | TYR | 459 | 81.488 | 58.470 | 89.903 | 1.00 | 13.80 |
| ATOM | 2836 | OH  | TYR | 459 | 80.340 | 57.885 | 89.442 | 1.00 | 13.75 |
| ATOM | 2837 | C   | TYR | 459 | 85.203 | 60.830 | 88.559 | 1.00 | 20.12 |
| ATOM | 2838 | O   | TYR | 459 | 85.135 | 59.896 | 87.758 | 1.00 | 22.54 |
| ATOM | 2839 | N   | LEU | 460 | 84.590 | 61.996 | 88.351 | 1.00 | 18.20 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2840 | CA  | LEU | 460 | 83.824 | 62.232 | 87.126 | 1.00 | 15.92 |
| ATOM | 2841 | CB  | LEU | 460 | 83.214 | 63.638 | 87.115 | 1.00 | 15.26 |
| ATOM | 2842 | CG  | LEU | 460 | 82.226 | 63.958 | 88.233 | 1.00 | 14.02 |
| ATOM | 2843 | CD1 | LEU | 460 | 81.818 | 65.404 | 88.150 | 1.00 | 12.72 |
| ATOM | 2844 | CD2 | LEU | 460 | 81.020 | 63.058 | 88.143 | 1.00 | 12.27 |
| ATOM | 2845 | C   | LEU | 460 | 84.735 | 62.052 | 85.916 | 1.00 | 15.36 |
| ATOM | 2846 | O   | LEU | 460 | 84.326 | 61.488 | 84.902 | 1.00 | 15.87 |
| ATOM | 2847 | N   | ILE | 461 | 85.970 | 62.542 | 86.027 | 1.00 | 16.13 |
| ATOM | 2848 | CA  | ILE | 461 | 86.968 | 62.428 | 84.952 | 1.00 | 15.25 |
| ATOM | 2849 | CB  | ILE | 461 | 88.288 | 63.144 | 85.336 | 1.00 | 14.67 |
| ATOM | 2850 | CG2 | ILE | 461 | 89.444 | 62.676 | 84.463 | 1.00 | 9.67  |
| ATOM | 2851 | CG1 | ILE | 461 | 88.103 | 64.667 | 85.247 | 1.00 | 17.36 |
| ATOM | 2852 | CD1 | ILE | 461 | 89.216 | 65.455 | 85.902 | 1.00 | 16.02 |
| ATOM | 2853 | C   | ILE | 461 | 87.233 | 60.951 | 84.640 | 1.00 | 15.38 |
| ATOM | 2854 | O   | ILE | 461 | 87.260 | 60.551 | 83.476 | 1.00 | 14.40 |
| ATOM | 2855 | N   | ALA | 462 | 87.395 | 60.143 | 85.683 | 1.00 | 14.36 |
| ATOM | 2856 | CA  | ALA | 462 | 87.622 | 58.722 | 85.500 | 1.00 | 15.50 |
| ATOM | 2857 | CB  | ALA | 462 | 87.932 | 58.070 | 86.830 | 1.00 | 14.39 |
| ATOM | 2858 | C   | ALA | 462 | 86.379 | 58.093 | 84.871 | 1.00 | 17.54 |
| ATOM | 2859 | O   | ALA | 462 | 86.473 | 57.338 | 83.902 | 1.00 | 19.03 |
| ATOM | 2860 | N   | GLY | 463 | 85.211 | 58.440 | 85.399 | 1.00 | 18.74 |
| ATOM | 2861 | CA  | GLY | 463 | 83.968 | 57.899 | 84.884 | 1.00 | 18.66 |
| ATOM | 2862 | C   | GLY | 463 | 83.795 | 58.158 | 83.403 | 1.00 | 19.50 |
| ATOM | 2863 | O   | GLY | 463 | 83.533 | 57.224 | 82.638 | 1.00 | 20.45 |
| ATOM | 2864 | N   | ILE | 464 | 83.992 | 59.410 | 82.992 | 1.00 | 18.46 |
| ATOM | 2865 | CA  | ILE | 464 | 83.845 | 59.797 | 81.594 | 1.00 | 18.81 |
| ATOM | 2866 | CB  | ILE | 464 | 84.106 | 61.298 | 81.371 | 1.00 | 16.10 |
| ATOM | 2867 | CG2 | ILE | 464 | 83.833 | 61.663 | 79.915 | 1.00 | 13.53 |
| ATOM | 2868 | CG1 | ILE | 464 | 83.196 | 62.129 | 82.270 | 1.00 | 12.34 |
| ATOM | 2869 | CD1 | ILE | 464 | 83.384 | 63.605 | 82.091 | 1.00 | 13.25 |
| ATOM | 2870 | C   | ILE | 464 | 84.791 | 59.007 | 80.703 | 1.00 | 21.38 |
| ATOM | 2871 | O   | ILE | 464 | 84.399 | 58.551 | 79.622 | 1.00 | 22.86 |
| ATOM | 2872 | N   | GLN | 465 | 86.024 | 58.826 | 81.177 | 1.00 | 20.93 |
| ATOM | 2873 | CA  | GLN | 465 | 87.050 | 58.085 | 80.443 | 1.00 | 19.17 |
| ATOM | 2874 | CB  | GLN | 465 | 88.360 | 58.086 | 81.216 | 1.00 | 16.09 |
| ATOM | 2875 | CG  | GLN | 465 | 89.063 | 59.411 | 81.190 | 1.00 | 13.01 |
| ATOM | 2876 | CD  | GLN | 465 | 90.394 | 59.341 | 81.867 | 1.00 | 12.51 |
| ATOM | 2877 | OE1 | GLN | 465 | 90.513 | 58.832 | 82.983 | 1.00 | 14.37 |
| ATOM | 2878 | NE2 | GLN | 465 | 91.418 | 59.829 | 81.193 | 1.00 | 16.53 |
| ATOM | 2879 | C   | GLN | 465 | 86.659 | 56.650 | 80.132 | 1.00 | 20.16 |
| ATOM | 2880 | O   | GLN | 465 | 86.902 | 56.159 | 79.027 | 1.00 | 22.29 |
| ATOM | 2881 | N   | HIS | 466 | 86.084 | 55.964 | 81.113 | 1.00 | 20.52 |
| ATOM | 2882 | CA  | HIS | 466 | 85.658 | 54.586 | 80.911 | 1.00 | 21.13 |
| ATOM | 2883 | CB  | HIS | 466 | 85.157 | 53.979 | 82.218 | 1.00 | 24.96 |
| ATOM | 2884 | CG  | HIS | 466 | 86.235 | 53.772 | 83.235 | 1.00 | 31.10 |
| ATOM | 2885 | CD2 | HIS | 466 | 86.820 | 54.632 | 84.100 | 1.00 | 30.04 |
| ATOM | 2886 | ND1 | HIS | 466 | 86.847 | 52.554 | 83.432 | 1.00 | 36.54 |
| ATOM | 2887 | CE1 | HIS | 466 | 87.763 | 52.673 | 84.374 | 1.00 | 37.26 |
| ATOM | 2888 | NE2 | HIS | 466 | 87.768 | 53.924 | 84.795 | 1.00 | 34.17 |
| ATOM | 2889 | C   | HIS | 466 | 84.565 | 54.536 | 79.846 | 1.00 | 21.83 |
| ATOM | 2890 | O   | HIS | 466 | 84.597 | 53.688 | 78.955 | 1.00 | 22.78 |
| ATOM | 2891 | N   | SER | 467 | 83.623 | 55.475 | 79.913 | 1.00 | 21.38 |
| ATOM | 2892 | CA  | SER | 467 | 82.541 | 55.528 | 78.939 | 1.00 | 18.96 |
| ATOM | 2893 | CB  | SER | 467 | 81.607 | 56.692 | 79.242 | 1.00 | 19.31 |
| ATOM | 2894 | OG  | SER | 467 | 80.530 | 56.712 | 78.336 | 1.00 | 19.95 |
| ATOM | 2895 | C   | SER | 467 | 83.124 | 55.653 | 77.539 | 1.00 | 17.24 |
| ATOM | 2896 | O   | SER | 467 | 82.725 | 54.928 | 76.639 | 1.00 | 20.25 |
| ATOM | 2897 | N   | CYS | 468 | 84.087 | 56.553 | 77.361 | 1.00 | 17.11 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2898 | CA  | CYS | 468 | 84.738 | 56.727 | 76.067 | 1.00 | 15.35 |
| ATOM | 2899 | CB  | CYS | 468 | 85.823 | 57.810 | 76.120 | 1.00 | 15.72 |
| ATOM | 2900 | SG  | CYS | 468 | 85.235 | 59.525 | 75.957 | 1.00 | 15.92 |
| ATOM | 2901 | C   | CYS | 468 | 85.366 | 55.413 | 75.649 | 1.00 | 15.52 |
| ATOM | 2902 | O   | CYS | 468 | 85.356 | 55.077 | 74.471 | 1.00 | 16.61 |
| ATOM | 2903 | N   | GLN | 469 | 85.894 | 54.656 | 76.609 | 1.00 | 14.54 |
| ATOM | 2904 | CA  | GLN | 469 | 86.505 | 53.376 | 76.285 | 1.00 | 14.20 |
| ATOM | 2905 | CB  | GLN | 469 | 87.231 | 52.779 | 77.480 | 1.00 | 12.53 |
| ATOM | 2906 | CG  | GLN | 469 | 87.852 | 51.442 | 77.120 | 1.00 | 10.20 |
| ATOM | 2907 | CD  | GLN | 469 | 88.499 | 50.763 | 78.303 | 1.00 | 10.73 |
| ATOM | 2908 | OE1 | GLN | 469 | 87.958 | 50.756 | 79.409 | 1.00 | 11.90 |
| ATOM | 2909 | NE2 | GLN | 469 | 89.665 | 50.171 | 78.071 | 1.00 | 11.04 |
| ATOM | 2910 | C   | GLN | 469 | 85.492 | 52.364 | 75.766 | 1.00 | 15.39 |
| ATOM | 2911 | O   | GLN | 469 | 85.708 | 51.734 | 74.736 | 1.00 | 17.75 |
| ATOM | 2912 | N   | ASP | 470 | 84.402 | 52.180 | 76.496 | 1.00 | 14.75 |
| ATOM | 2913 | CA  | ASP | 470 | 83.384 | 51.240 | 76.078 | 1.00 | 14.71 |
| ATOM | 2914 | CB  | ASP | 470 | 82.213 | 51.243 | 77.059 | 1.00 | 14.31 |
| ATOM | 2915 | CG  | ASP | 470 | 82.524 | 50.507 | 78.352 | 1.00 | 16.63 |
| ATOM | 2916 | OD1 | ASP | 470 | 83.543 | 49.784 | 78.426 | 1.00 | 13.27 |
| ATOM | 2917 | OD2 | ASP | 470 | 81.720 | 50.650 | 79.299 | 1.00 | 17.13 |
| ATOM | 2918 | C   | ASP | 470 | 82.890 | 51.580 | 74.679 | 1.00 | 15.71 |
| ATOM | 2919 | O   | ASP | 470 | 82.766 | 50.701 | 73.826 | 1.00 | 15.68 |
| ATOM | 2920 | N   | ILE | 471 | 82.656 | 52.864 | 74.427 | 1.00 | 15.09 |
| ATOM | 2921 | CA  | ILE | 471 | 82.164 | 53.276 | 73.121 | 1.00 | 17.16 |
| ATOM | 2922 | CB  | ILE | 471 | 81.410 | 54.644 | 73.178 | 1.00 | 15.42 |
| ATOM | 2923 | CG2 | ILE | 471 | 80.441 | 54.662 | 74.361 | 1.00 | 12.68 |
| ATOM | 2924 | CG1 | ILE | 471 | 82.379 | 55.815 | 73.305 | 1.00 | 16.88 |
| ATOM | 2925 | CD1 | ILE | 471 | 81.675 | 57.153 | 73.500 | 1.00 | 19.09 |
| ATOM | 2926 | C   | ILE | 471 | 83.245 | 53.261 | 72.033 | 1.00 | 19.70 |
| ATOM | 2927 | O   | ILE | 471 | 82.945 | 53.462 | 70.855 | 1.00 | 21.58 |
| ATOM | 2928 | N   | GLY | 472 | 84.488 | 52.986 | 72.429 | 1.00 | 18.31 |
| ATOM | 2929 | CA  | GLY | 472 | 85.594 | 52.915 | 71.484 | 1.00 | 17.02 |
| ATOM | 2930 | C   | GLY | 472 | 86.170 | 54.225 | 70.983 | 1.00 | 17.61 |
| ATOM | 2931 | O   | GLY | 472 | 86.616 | 54.308 | 69.838 | 1.00 | 19.06 |
| ATOM | 2932 | N   | ALA | 473 | 86.203 | 55.236 | 71.846 | 1.00 | 18.13 |
| ATOM | 2933 | CA  | ALA | 473 | 86.735 | 56.552 | 71.490 | 1.00 | 16.93 |
| ATOM | 2934 | CB  | ALA | 473 | 85.629 | 57.580 | 71.524 | 1.00 | 15.29 |
| ATOM | 2935 | C   | ALA | 473 | 87.870 | 56.968 | 72.428 | 1.00 | 17.85 |
| ATOM | 2936 | O   | ALA | 473 | 87.718 | 56.945 | 73.651 | 1.00 | 19.09 |
| ATOM | 2937 | N   | LYS | 474 | 89.010 | 57.325 | 71.847 | 1.00 | 16.96 |
| ATOM | 2938 | CA  | LYS | 474 | 90.182 | 57.748 | 72.611 | 1.00 | 17.79 |
| ATOM | 2939 | CB  | LYS | 474 | 91.462 | 57.563 | 71.789 | 1.00 | 21.65 |
| ATOM | 2940 | CG  | LYS | 474 | 91.817 | 56.137 | 71.397 | 1.00 | 31.55 |
| ATOM | 2941 | CD  | LYS | 474 | 93.090 | 56.130 | 70.525 | 1.00 | 40.40 |
| ATOM | 2942 | CE  | LYS | 474 | 93.447 | 54.741 | 69.987 | 1.00 | 44.48 |
| ATOM | 2943 | NZ  | LYS | 474 | 93.906 | 53.804 | 71.052 | 1.00 | 47.47 |
| ATOM | 2944 | C   | LYS | 474 | 90.121 | 59.202 | 73.065 | 1.00 | 15.79 |
| ATOM | 2945 | O   | LYS | 474 | 90.995 | 59.643 | 73.801 | 1.00 | 15.96 |
| ATOM | 2946 | N   | SER | 475 | 89.118 | 59.952 | 72.614 | 1.00 | 14.00 |
| ATOM | 2947 | CA  | SER | 475 | 88.987 | 61.356 | 72.991 | 1.00 | 13.63 |
| ATOM | 2948 | CB  | SER | 475 | 89.987 | 62.207 | 72.213 | 1.00 | 12.89 |
| ATOM | 2949 | OG  | SER | 475 | 89.804 | 62.056 | 70.815 | 1.00 | 11.85 |
| ATOM | 2950 | C   | SER | 475 | 87.590 | 61.892 | 72.727 | 1.00 | 14.26 |
| ATOM | 2951 | O   | SER | 475 | 86.876 | 61.379 | 71.867 | 1.00 | 15.62 |
| ATOM | 2952 | N   | LEU | 476 | 87.222 | 62.960 | 73.429 | 1.00 | 15.53 |
| ATOM | 2953 | CA  | LEU | 476 | 85.903 | 63.572 | 73.258 | 1.00 | 16.54 |
| ATOM | 2954 | CB  | LEU | 476 | 85.707 | 64.745 | 74.226 | 1.00 | 12.36 |
| ATOM | 2955 | CG  | LEU | 476 | 85.603 | 64.398 | 75.718 | 1.00 | 11.06 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2956 | CD1 | LEU | 476 | 85.238 | 65.641 | 76.512 | 1.00 | 6.39  |
| ATOM | 2957 | CD2 | LEU | 476 | 84.557 | 63.318 | 75.932 | 1.00 | 9.52  |
| ATOM | 2958 | C   | LEU | 476 | 85.736 | 64.036 | 71.823 | 1.00 | 17.37 |
| ATOM | 2959 | O   | LEU | 476 | 84.658 | 63.935 | 71.238 | 1.00 | 19.71 |
| ATOM | 2960 | N   | THR | 477 | 86.828 | 64.512 | 71.244 | 1.00 | 19.45 |
| ATOM | 2961 | CA  | THR | 477 | 86.835 | 64.971 | 69.867 | 1.00 | 20.10 |
| ATOM | 2962 | CB  | THR | 477 | 88.227 | 65.479 | 69.481 | 1.00 | 20.18 |
| ATOM | 2963 | OG1 | THR | 477 | 88.655 | 66.456 | 70.438 | 1.00 | 20.52 |
| ATOM | 2964 | CG2 | THR | 477 | 88.202 | 66.085 | 68.088 | 1.00 | 21.34 |
| ATOM | 2965 | C   | THR | 477 | 86.473 | 63.801 | 68.956 | 1.00 | 20.32 |
| ATOM | 2966 | O   | THR | 477 | 85.716 | 63.962 | 68.004 | 1.00 | 20.43 |
| ATOM | 2967 | N   | GLN | 478 | 87.002 | 62.623 | 69.276 | 1.00 | 19.47 |
| ATOM | 2968 | CA  | GLN | 478 | 86.735 | 61.430 | 68.485 | 1.00 | 19.30 |
| ATOM | 2969 | CB  | GLN | 478 | 87.649 | 60.278 | 68.902 | 1.00 | 20.23 |
| ATOM | 2970 | CG  | GLN | 478 | 87.681 | 59.135 | 67.896 | 1.00 | 21.67 |
| ATOM | 2971 | CD  | GLN | 478 | 88.536 | 57.970 | 68.345 | 1.00 | 22.44 |
| ATOM | 2972 | OE1 | GLN | 478 | 89.243 | 58.049 | 69.343 | 1.00 | 22.21 |
| ATOM | 2973 | NE2 | GLN | 478 | 88.457 | 56.871 | 67.619 | 1.00 | 25.65 |
| ATOM | 2974 | C   | GLN | 478 | 85.284 | 61.005 | 68.635 | 1.00 | 18.53 |
| ATOM | 2975 | O   | GLN | 478 | 84.634 | 60.653 | 67.646 | 1.00 | 20.45 |
| ATOM | 2976 | N   | VAL | 479 | 84.774 | 61.057 | 69.862 | 1.00 | 16.40 |
| ATOM | 2977 | CA  | VAL | 479 | 83.390 | 60.676 | 70.122 | 1.00 | 15.90 |
| ATOM | 2978 | CB  | VAL | 479 | 82.986 | 60.898 | 71.597 | 1.00 | 15.74 |
| ATOM | 2979 | CG1 | VAL | 479 | 81.591 | 60.352 | 71.849 | 1.00 | 13.93 |
| ATOM | 2980 | CG2 | VAL | 479 | 83.965 | 60.205 | 72.515 | 1.00 | 17.75 |
| ATOM | 2981 | C   | VAL | 479 | 82.436 | 61.439 | 69.207 | 1.00 | 14.57 |
| ATOM | 2982 | O   | VAL | 479 | 81.536 | 60.843 | 68.613 | 1.00 | 14.93 |
| ATOM | 2983 | N   | ARG | 480 | 82.649 | 62.743 | 69.059 | 1.00 | 14.86 |
| ATOM | 2984 | CA  | ARG | 480 | 81.788 | 63.537 | 68.180 | 1.00 | 14.83 |
| ATOM | 2985 | CB  | ARG | 480 | 82.017 | 65.021 | 68.390 | 1.00 | 13.38 |
| ATOM | 2986 | CG  | ARG | 480 | 81.403 | 65.513 | 69.661 | 1.00 | 13.20 |
| ATOM | 2987 | CD  | ARG | 480 | 81.994 | 66.825 | 70.054 | 1.00 | 17.86 |
| ATOM | 2988 | NE  | ARG | 480 | 82.330 | 66.787 | 71.468 | 1.00 | 27.35 |
| ATOM | 2989 | CZ  | ARG | 480 | 83.501 | 67.159 | 71.967 | 1.00 | 31.62 |
| ATOM | 2990 | NH1 | ARG | 480 | 84.459 | 67.606 | 71.162 | 1.00 | 30.46 |
| ATOM | 2991 | NH2 | ARG | 480 | 83.718 | 67.065 | 73.273 | 1.00 | 35.55 |
| ATOM | 2992 | C   | ARG | 480 | 81.925 | 63.179 | 66.706 | 1.00 | 13.45 |
| ATOM | 2993 | O   | ARG | 480 | 80.930 | 63.121 | 65.986 | 1.00 | 13.13 |
| ATOM | 2994 | N   | ALA | 481 | 83.145 | 62.909 | 66.260 | 1.00 | 13.31 |
| ATOM | 2995 | CA  | ALA | 481 | 83.369 | 62.534 | 64.869 | 1.00 | 15.17 |
| ATOM | 2996 | CB  | ALA | 481 | 84.844 | 62.311 | 64.610 | 1.00 | 16.26 |
| ATOM | 2997 | C   | ALA | 481 | 82.590 | 61.256 | 64.590 | 1.00 | 16.54 |
| ATOM | 2998 | O   | ALA | 481 | 81.852 | 61.177 | 63.605 | 1.00 | 18.67 |
| ATOM | 2999 | N   | MET | 482 | 82.752 | 60.265 | 65.465 | 1.00 | 15.36 |
| ATOM | 3000 | CA  | MET | 482 | 82.057 | 58.985 | 65.350 | 1.00 | 15.54 |
| ATOM | 3001 | CB  | MET | 482 | 82.430 | 58.061 | 66.512 | 1.00 | 14.12 |
| ATOM | 3002 | CG  | MET | 482 | 83.821 | 57.466 | 66.432 | 1.00 | 14.38 |
| ATOM | 3003 | SD  | MET | 482 | 84.228 | 56.501 | 67.895 | 1.00 | 19.57 |
| ATOM | 3004 | CE  | MET | 482 | 83.309 | 55.013 | 67.579 | 1.00 | 5.26  |
| ATOM | 3005 | C   | MET | 482 | 80.544 | 59.175 | 65.333 | 1.00 | 17.70 |
| ATOM | 3006 | O   | MET | 482 | 79.835 | 58.490 | 64.597 | 1.00 | 21.04 |
| ATOM | 3007 | N   | MET | 483 | 80.045 | 60.101 | 66.142 | 1.00 | 17.24 |
| ATOM | 3008 | CA  | MET | 483 | 78.617 | 60.350 | 66.190 | 1.00 | 17.79 |
| ATOM | 3009 | CB  | MET | 483 | 78.254 | 61.118 | 67.467 | 1.00 | 20.77 |
| ATOM | 3010 | CG  | MET | 483 | 78.076 | 62.603 | 67.310 | 1.00 | 25.75 |
| ATOM | 3011 | SD  | MET | 483 | 76.433 | 62.978 | 66.748 | 1.00 | 27.11 |
| ATOM | 3012 | CE  | MET | 483 | 76.244 | 64.529 | 67.464 | 1.00 | 28.07 |
| ATOM | 3013 | C   | MET | 483 | 78.141 | 61.057 | 64.921 | 1.00 | 17.84 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3014 | O   | MET | 483 | 77.122 | 60.677 | 64.347 | 1.00 | 18.55 |
| ATOM | 3015 | N   | TYR | 484 | 78.907 | 62.034 | 64.442 | 1.00 | 18.23 |
| ATOM | 3016 | CA  | TYR | 484 | 78.553 | 62.769 | 63.221 | 1.00 | 18.32 |
| ATOM | 3017 | CB  | TYR | 484 | 79.324 | 64.084 | 63.136 | 1.00 | 13.90 |
| ATOM | 3018 | CG  | TYR | 484 | 78.821 | 65.154 | 64.062 | 1.00 | 12.61 |
| ATOM | 3019 | CD1 | TYR | 484 | 77.504 | 65.594 | 64.000 | 1.00 | 10.69 |
| ATOM | 3020 | CE1 | TYR | 484 | 77.044 | 66.605 | 64.854 | 1.00 | 11.90 |
| ATOM | 3021 | CD2 | TYR | 484 | 79.670 | 65.740 | 64.999 | 1.00 | 13.80 |
| ATOM | 3022 | CE2 | TYR | 484 | 79.228 | 66.741 | 65.851 | 1.00 | 10.55 |
| ATOM | 3023 | CZ  | TYR | 484 | 77.916 | 67.169 | 65.772 | 1.00 | 8.99  |
| ATOM | 3024 | OH  | TYR | 484 | 77.503 | 68.179 | 66.596 | 1.00 | 7.99  |
| ATOM | 3025 | C   | TYR | 484 | 78.767 | 61.985 | 61.923 | 1.00 | 19.94 |
| ATOM | 3026 | O   | TYR | 484 | 78.141 | 62.282 | 60.902 | 1.00 | 22.03 |
| ATOM | 3027 | N   | SER | 485 | 79.671 | 61.012 | 61.951 | 1.00 | 18.19 |
| ATOM | 3028 | CA  | SER | 485 | 79.947 | 60.192 | 60.775 | 1.00 | 18.62 |
| ATOM | 3029 | CB  | SER | 485 | 81.329 | 59.558 | 60.882 | 1.00 | 21.82 |
| ATOM | 3030 | OG  | SER | 485 | 81.401 | 58.715 | 62.023 | 1.00 | 27.56 |
| ATOM | 3031 | C   | SER | 485 | 78.927 | 59.074 | 60.659 | 1.00 | 18.30 |
| ATOM | 3032 | O   | SER | 485 | 78.865 | 58.388 | 59.639 | 1.00 | 19.04 |
| ATOM | 3033 | N   | GLY | 486 | 78.200 | 58.840 | 61.747 | 1.00 | 17.81 |
| ATOM | 3034 | CA  | GLY | 486 | 77.204 | 57.789 | 61.774 | 1.00 | 14.51 |
| ATOM | 3035 | C   | GLY | 486 | 77.740 | 56.579 | 62.510 | 1.00 | 13.19 |
| ATOM | 3036 | O   | GLY | 486 | 76.973 | 55.791 | 63.042 | 1.00 | 15.77 |
| ATOM | 3037 | N   | GLU | 487 | 79.061 | 56.462 | 62.589 | 1.00 | 11.32 |
| ATOM | 3038 | CA  | GLU | 487 | 79.705 | 55.335 | 63.251 | 1.00 | 10.96 |
| ATOM | 3039 | CB  | GLU | 487 | 81.213 | 55.561 | 63.311 | 1.00 | 12.35 |
| ATOM | 3040 | CG  | GLU | 487 | 81.980 | 54.438 | 63.999 | 1.00 | 11.26 |
| ATOM | 3041 | CD  | GLU | 487 | 83.483 | 54.632 | 63.984 | 1.00 | 12.67 |
| ATOM | 3042 | OE1 | GLU | 487 | 83.978 | 55.618 | 63.383 | 1.00 | 14.49 |
| ATOM | 3043 | OE2 | GLU | 487 | 84.177 | 53.785 | 64.574 | 1.00 | 15.10 |
| ATOM | 3044 | C   | GLU | 487 | 79.196 | 54.984 | 64.650 | 1.00 | 11.80 |
| ATOM | 3045 | O   | GLU | 487 | 79.117 | 53.806 | 65.002 | 1.00 | 10.47 |
| ATOM | 3046 | N   | LEU | 488 | 78.915 | 55.999 | 65.464 | 1.00 | 11.14 |
| ATOM | 3047 | CA  | LEU | 488 | 78.433 | 55.769 | 66.819 | 1.00 | 9.95  |
| ATOM | 3048 | CB  | LEU | 488 | 78.671 | 57.006 | 67.691 | 1.00 | 9.92  |
| ATOM | 3049 | CG  | LEU | 488 | 78.505 | 56.890 | 69.213 | 1.00 | 10.98 |
| ATOM | 3050 | CD1 | LEU | 488 | 79.352 | 55.770 | 69.767 | 1.00 | 13.79 |
| ATOM | 3051 | CD2 | LEU | 488 | 78.912 | 58.186 | 69.869 | 1.00 | 10.11 |
| ATOM | 3052 | C   | LEU | 488 | 76.951 | 55.448 | 66.731 | 1.00 | 12.30 |
| ATOM | 3053 | O   | LEU | 488 | 76.206 | 55.132 | 66.034 | 1.00 | 13.80 |
| ATOM | 3054 | N   | LYS | 489 | 76.529 | 54.385 | 67.407 | 1.00 | 12.49 |
| ATOM | 3055 | CA  | LYS | 489 | 75.133 | 53.983 | 67.385 | 1.00 | 9.72  |
| ATOM | 3056 | CB  | LYS | 489 | 75.013 | 52.534 | 66.927 | 1.00 | 7.65  |
| ATOM | 3057 | CG  | LYS | 489 | 75.553 | 52.273 | 65.542 | 1.00 | 6.90  |
| ATOM | 3058 | CD  | LYS | 489 | 74.793 | 53.048 | 64.486 | 1.00 | 8.74  |
| ATOM | 3059 | CE  | LYS | 489 | 75.343 | 52.755 | 63.105 | 1.00 | 8.65  |
| ATOM | 3060 | NZ  | LYS | 489 | 74.236 | 52.827 | 62.110 | 1.00 | 21.71 |
| ATOM | 3061 | C   | LYS | 489 | 74.480 | 54.143 | 68.744 | 1.00 | 10.66 |
| ATOM | 3062 | O   | LYS | 489 | 75.137 | 54.063 | 69.777 | 1.00 | 10.17 |
| ATOM | 3063 | N   | PHE | 490 | 73.169 | 54.332 | 68.730 | 1.00 | 11.10 |
| ATOM | 3064 | CA  | PHE | 490 | 72.391 | 54.500 | 69.941 | 1.00 | 10.52 |
| ATOM | 3065 | CB  | PHE | 490 | 71.884 | 55.947 | 70.063 | 1.00 | 10.19 |
| ATOM | 3066 | CG  | PHE | 490 | 72.968 | 56.987 | 69.999 | 1.00 | 11.62 |
| ATOM | 3067 | CD1 | PHE | 490 | 73.510 | 57.375 | 68.784 | 1.00 | 10.59 |
| ATOM | 3068 | CD2 | PHE | 490 | 73.450 | 57.576 | 71.161 | 1.00 | 14.71 |
| ATOM | 3069 | CE1 | PHE | 490 | 74.513 | 58.332 | 68.728 | 1.00 | 10.01 |
| ATOM | 3070 | CE2 | PHE | 490 | 74.456 | 58.537 | 71.113 | 1.00 | 11.23 |
| ATOM | 3071 | CZ  | PHE | 490 | 74.987 | 58.911 | 69.899 | 1.00 | 8.86  |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3072 | C   | PHE | 490 | 71.186 | 53.585 | 69.808 | 1.00 | 12.95 |
| ATOM | 3073 | O   | PHE | 490 | 70.974 | 52.955 | 68.754 | 1.00 | 12.71 |
| ATOM | 3074 | N   | GLU | 491 | 70.404 | 53.523 | 70.883 | 1.00 | 13.66 |
| ATOM | 3075 | CA  | GLU | 491 | 69.174 | 52.742 | 70.943 | 1.00 | 14.24 |
| ATOM | 3076 | CB  | GLU | 491 | 69.480 | 51.260 | 71.171 | 1.00 | 14.20 |
| ATOM | 3077 | CG  | GLU | 491 | 68.245 | 50.402 | 71.226 | 1.00 | 11.29 |
| ATOM | 3078 | CD  | GLU | 491 | 68.526 | 48.976 | 70.870 | 1.00 | 12.52 |
| ATOM | 3079 | OE1 | GLU | 491 | 68.577 | 48.667 | 69.662 | 1.00 | 14.42 |
| ATOM | 3080 | OE2 | GLU | 491 | 68.704 | 48.168 | 71.796 | 1.00 | 12.45 |
| ATOM | 3081 | C   | GLU | 491 | 68.252 | 53.288 | 72.050 | 1.00 | 15.42 |
| ATOM | 3082 | O   | GLU | 491 | 68.698 | 53.544 | 73.177 | 1.00 | 15.37 |
| ATOM | 3083 | N   | LYS | 492 | 66.989 | 53.521 | 71.704 | 1.00 | 15.56 |
| ATOM | 3084 | CA  | LYS | 492 | 66.013 | 54.038 | 72.658 | 1.00 | 16.28 |
| ATOM | 3085 | CB  | LYS | 492 | 64.674 | 54.295 | 71.970 | 1.00 | 16.97 |
| ATOM | 3086 | CG  | LYS | 492 | 64.727 | 55.368 | 70.906 | 1.00 | 22.04 |
| ATOM | 3087 | CD  | LYS | 492 | 63.471 | 55.376 | 70.050 | 1.00 | 30.69 |
| ATOM | 3088 | CE  | LYS | 492 | 62.229 | 55.692 | 70.876 | 1.00 | 40.54 |
| ATOM | 3089 | NZ  | LYS | 492 | 60.981 | 55.643 | 70.060 | 1.00 | 44.71 |
| ATOM | 3090 | C   | LYS | 492 | 65.797 | 53.034 | 73.772 | 1.00 | 16.62 |
| ATOM | 3091 | O   | LYS | 492 | 65.940 | 51.834 | 73.562 | 1.00 | 18.55 |
| ATOM | 3092 | N   | ARG | 493 | 65.445 | 53.534 | 74.950 | 1.00 | 17.23 |
| ATOM | 3093 | CA  | ARG | 493 | 65.184 | 52.698 | 76.114 | 1.00 | 15.40 |
| ATOM | 3094 | CB  | ARG | 493 | 66.068 | 53.110 | 77.292 | 1.00 | 12.64 |
| ATOM | 3095 | CG  | ARG | 493 | 67.464 | 52.564 | 77.237 | 1.00 | 16.13 |
| ATOM | 3096 | CD  | ARG | 493 | 68.060 | 52.481 | 78.616 | 1.00 | 14.05 |
| ATOM | 3097 | NE  | ARG | 493 | 68.213 | 53.788 | 79.232 | 1.00 | 15.84 |
| ATOM | 3098 | CZ  | ARG | 493 | 68.714 | 53.978 | 80.450 | 1.00 | 19.92 |
| ATOM | 3099 | NH1 | ARG | 493 | 69.108 | 52.940 | 81.179 | 1.00 | 17.89 |
| ATOM | 3100 | NH2 | ARG | 493 | 68.816 | 55.206 | 80.947 | 1.00 | 20.74 |
| ATOM | 3101 | C   | ARG | 493 | 63.741 | 52.822 | 76.559 | 1.00 | 16.72 |
| ATOM | 3102 | O   | ARG | 493 | 63.316 | 53.891 | 76.991 | 1.00 | 17.93 |
| ATOM | 3103 | N   | THR | 494 | 62.972 | 51.747 | 76.444 | 1.00 | 17.78 |
| ATOM | 3104 | CA  | THR | 494 | 61.593 | 51.785 | 76.911 | 1.00 | 18.02 |
| ATOM | 3105 | CB  | THR | 494 | 60.873 | 50.472 | 76.627 | 1.00 | 16.97 |
| ATOM | 3106 | OG1 | THR | 494 | 61.699 | 49.381 | 77.047 | 1.00 | 19.57 |
| ATOM | 3107 | CG2 | THR | 494 | 60.573 | 50.333 | 75.155 | 1.00 | 17.62 |
| ATOM | 3108 | C   | THR | 494 | 61.700 | 51.959 | 78.425 | 1.00 | 19.69 |
| ATOM | 3109 | O   | THR | 494 | 62.782 | 51.780 | 78.998 | 1.00 | 22.59 |
| ATOM | 3110 | N   | SER | 495 | 60.602 | 52.311 | 79.079 | 1.00 | 19.02 |
| ATOM | 3111 | CA  | SER | 495 | 60.608 | 52.496 | 80.523 | 1.00 | 18.50 |
| ATOM | 3112 | CB  | SER | 495 | 59.226 | 52.910 | 80.981 | 1.00 | 24.80 |
| ATOM | 3113 | OG  | SER | 495 | 58.776 | 53.997 | 80.183 | 1.00 | 39.46 |
| ATOM | 3114 | C   | SER | 495 | 61.072 | 51.239 | 81.254 | 1.00 | 18.35 |
| ATOM | 3115 | O   | SER | 495 | 61.835 | 51.326 | 82.214 | 1.00 | 17.67 |
| ATOM | 3116 | N   | SER | 496 | 60.631 | 50.071 | 80.784 | 1.00 | 17.30 |
| ATOM | 3117 | CA  | SER | 496 | 61.042 | 48.802 | 81.378 | 1.00 | 16.26 |
| ATOM | 3118 | CB  | SER | 496 | 60.331 | 47.633 | 80.697 | 1.00 | 15.19 |
| ATOM | 3119 | OG  | SER | 496 | 58.931 | 47.811 | 80.695 | 1.00 | 20.72 |
| ATOM | 3120 | C   | SER | 496 | 62.545 | 48.665 | 81.156 | 1.00 | 17.45 |
| ATOM | 3121 | O   | SER | 496 | 63.272 | 48.164 | 82.023 | 1.00 | 17.49 |
| ATOM | 3122 | N   | ALA | 497 | 62.998 | 49.116 | 79.987 | 1.00 | 16.53 |
| ATOM | 3123 | CA  | ALA | 497 | 64.403 | 49.069 | 79.625 | 1.00 | 16.21 |
| ATOM | 3124 | CB  | ALA | 497 | 64.582 | 49.440 | 78.172 | 1.00 | 15.16 |
| ATOM | 3125 | C   | ALA | 497 | 65.211 | 50.000 | 80.522 | 1.00 | 17.84 |
| ATOM | 3126 | O   | ALA | 497 | 66.365 | 49.712 | 80.842 | 1.00 | 19.41 |
| ATOM | 3127 | N   | GLN | 498 | 64.603 | 51.109 | 80.938 | 1.00 | 18.51 |
| ATOM | 3128 | CA  | GLN | 498 | 65.268 | 52.067 | 81.829 | 1.00 | 18.22 |
| ATOM | 3129 | CB  | GLN | 498 | 64.520 | 53.391 | 81.838 | 1.00 | 14.72 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3130 | CG  | GLN | 498 | 64.614 | 54.155 | 80.542 | 1.00 | 16.17 |
| ATOM | 3131 | CD  | GLN | 498 | 63.737 | 55.389 | 80.552 | 1.00 | 21.61 |
| ATOM | 3132 | OE1 | GLN | 498 | 63.701 | 56.134 | 81.530 | 1.00 | 23.31 |
| ATOM | 3133 | NE2 | GLN | 498 | 63.000 | 55.597 | 79.471 | 1.00 | 25.52 |
| ATOM | 3134 | C   | GLN | 498 | 65.319 | 51.510 | 83.248 | 1.00 | 19.49 |
| ATOM | 3135 | O   | GLN | 498 | 66.288 | 51.728 | 83.973 | 1.00 | 21.42 |
| ATOM | 3136 | N   | VAL | 499 | 64.258 | 50.802 | 83.633 | 1.00 | 19.64 |
| ATOM | 3137 | CA  | VAL | 499 | 64.137 | 50.166 | 84.945 | 1.00 | 20.58 |
| ATOM | 3138 | CB  | VAL | 499 | 62.712 | 49.567 | 85.124 | 1.00 | 24.21 |
| ATOM | 3139 | CG1 | VAL | 499 | 62.670 | 48.559 | 86.284 | 1.00 | 26.96 |
| ATOM | 3140 | CG2 | VAL | 499 | 61.714 | 50.682 | 85.364 | 1.00 | 23.58 |
| ATOM | 3141 | C   | VAL | 499 | 65.166 | 49.042 | 85.060 | 1.00 | 20.51 |
| ATOM | 3142 | O   | VAL | 499 | 65.775 | 48.828 | 86.117 | 1.00 | 17.74 |
| ATOM | 3143 | N   | GLU | 500 | 65.318 | 48.310 | 83.960 | 1.00 | 22.30 |
| ATOM | 3144 | CA  | GLU | 500 | 66.255 | 47.202 | 83.871 | 1.00 | 22.71 |
| ATOM | 3145 | CB  | GLU | 500 | 66.028 | 46.436 | 82.574 | 1.00 | 17.71 |
| ATOM | 3146 | CG  | GLU | 500 | 67.069 | 45.379 | 82.317 | 1.00 | 17.26 |
| ATOM | 3147 | CD  | GLU | 500 | 66.915 | 44.749 | 80.966 | 1.00 | 21.30 |
| ATOM | 3148 | OE1 | GLU | 500 | 66.357 | 43.633 | 80.903 | 1.00 | 24.96 |
| ATOM | 3149 | OE2 | GLU | 500 | 67.346 | 45.365 | 79.965 | 1.00 | 21.01 |
| ATOM | 3150 | C   | GLU | 500 | 67.692 | 47.709 | 83.913 | 1.00 | 25.21 |
| ATOM | 3151 | O   | GLU | 500 | 68.579 | 47.027 | 84.432 | 1.00 | 27.22 |
| ATOM | 3152 | N   | GLY | 501 | 67.912 | 48.879 | 83.316 | 1.00 | 24.95 |
| ATOM | 3153 | CA  | GLY | 501 | 69.230 | 49.484 | 83.285 | 1.00 | 23.31 |
| ATOM | 3154 | C   | GLY | 501 | 69.723 | 49.914 | 84.653 | 1.00 | 23.43 |
| ATOM | 3155 | O   | GLY | 501 | 70.931 | 49.967 | 84.885 | 1.00 | 24.54 |
| ATOM | 3156 | N   | GLY | 502 | 68.801 | 50.268 | 85.544 | 1.00 | 22.98 |
| ATOM | 3157 | CA  | GLY | 502 | 69.185 | 50.676 | 86.886 | 1.00 | 21.16 |
| ATOM | 3158 | C   | GLY | 502 | 69.157 | 49.489 | 87.833 | 1.00 | 20.14 |
| ATOM | 3159 | O   | GLY | 502 | 68.977 | 48.347 | 87.404 | 1.00 | 19.33 |
| ATOM | 3160 | N   | VAL | 503 | 69.330 | 49.747 | 89.123 | 1.00 | 18.98 |
| ATOM | 3161 | CA  | VAL | 503 | 69.304 | 48.679 | 90.113 | 1.00 | 19.85 |
| ATOM | 3162 | CB  | VAL | 503 | 69.848 | 49.145 | 91.468 | 1.00 | 15.03 |
| ATOM | 3163 | CG1 | VAL | 503 | 69.691 | 48.039 | 92.503 | 1.00 | 15.02 |
| ATOM | 3164 | CG2 | VAL | 503 | 71.291 | 49.559 | 91.329 | 1.00 | 12.67 |
| ATOM | 3165 | C   | VAL | 503 | 67.876 | 48.185 | 90.316 | 1.00 | 24.02 |
| ATOM | 3166 | O   | VAL | 503 | 66.956 | 48.976 | 90.545 | 1.00 | 25.36 |
| ATOM | 3167 | N   | HIS | 504 | 67.697 | 46.870 | 90.252 | 1.00 | 26.21 |
| ATOM | 3168 | CA  | HIS | 504 | 66.383 | 46.270 | 90.443 | 1.00 | 27.57 |
| ATOM | 3169 | CB  | HIS | 504 | 65.643 | 46.117 | 89.102 | 1.00 | 23.86 |
| ATOM | 3170 | CG  | HIS | 504 | 66.377 | 45.298 | 88.078 | 1.00 | 21.19 |
| ATOM | 3171 | CD2 | HIS | 504 | 67.136 | 45.667 | 87.021 | 1.00 | 19.48 |
| ATOM | 3172 | ND1 | HIS | 504 | 66.340 | 43.919 | 88.056 | 1.00 | 16.78 |
| ATOM | 3173 | CE1 | HIS | 504 | 67.044 | 43.478 | 87.029 | 1.00 | 11.24 |
| ATOM | 3174 | NE2 | HIS | 504 | 67.539 | 44.517 | 86.387 | 1.00 | 12.99 |
| ATOM | 3175 | C   | HIS | 504 | 66.492 | 44.922 | 91.135 | 1.00 | 29.67 |
| ATOM | 3176 | O   | HIS | 504 | 67.588 | 44.401 | 91.334 | 1.00 | 29.30 |
| ATOM | 3177 | N   | SER | 505 | 65.347 | 44.407 | 91.567 | 1.00 | 31.87 |
| ATOM | 3178 | CA  | SER | 505 | 65.255 | 43.100 | 92.201 | 1.00 | 34.64 |
| ATOM | 3179 | CB  | SER | 505 | 65.572 | 42.008 | 91.169 | 1.00 | 36.20 |
| ATOM | 3180 | OG  | SER | 505 | 64.746 | 42.151 | 90.016 | 1.00 | 38.33 |
| ATOM | 3181 | C   | SER | 505 | 66.070 | 42.882 | 93.476 | 1.00 | 36.15 |
| ATOM | 3182 | O   | SER | 505 | 66.369 | 41.735 | 93.837 | 1.00 | 38.12 |
| ATOM | 3183 | N   | LEU | 506 | 66.411 | 43.960 | 94.172 | 1.00 | 35.02 |
| ATOM | 3184 | CA  | LEU | 506 | 67.161 | 43.825 | 95.415 | 1.00 | 35.93 |
| ATOM | 3185 | CB  | LEU | 506 | 68.354 | 44.779 | 95.454 | 1.00 | 33.98 |
| ATOM | 3186 | CG  | LEU | 506 | 69.443 | 44.537 | 94.419 | 1.00 | 32.60 |
| ATOM | 3187 | CD1 | LEU | 506 | 70.627 | 45.416 | 94.745 | 1.00 | 31.60 |

FIGURE 1 (CONT.)

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 3188 | CD2 | LEU | 506 | 69.842 | 43.068 | 94.416  | 1.00 | 30.24 |
| ATOM | 3189 | C   | LEU | 506 | 66.245 | 44.112 | 96.591  | 1.00 | 37.40 |
| ATOM | 3190 | O   | LEU | 506 | 65.313 | 44.911 | 96.478  | 1.00 | 39.36 |
| ATOM | 3191 | N   | HIS | 507 | 66.475 | 43.433 | 97.707  | 1.00 | 37.50 |
| ATOM | 3192 | CA  | HIS | 507 | 65.666 | 43.667 | 98.888  | 1.00 | 36.26 |
| ATOM | 3193 | CB  | HIS | 507 | 65.771 | 42.502 | 99.863  | 1.00 | 36.36 |
| ATOM | 3194 | CG  | HIS | 507 | 64.968 | 42.689 | 101.107 | 1.00 | 39.58 |
| ATOM | 3195 | CD2 | HIS | 507 | 63.726 | 42.268 | 101.439 | 1.00 | 40.11 |
| ATOM | 3196 | ND1 | HIS | 507 | 65.426 | 43.420 | 102.184 | 1.00 | 41.90 |
| ATOM | 3197 | CE1 | HIS | 507 | 64.501 | 43.442 | 103.127 | 1.00 | 42.56 |
| ATOM | 3198 | NE2 | HIS | 507 | 63.458 | 42.753 | 102.700 | 1.00 | 44.44 |
| ATOM | 3199 | C   | HIS | 507 | 66.169 | 44.951 | 99.535  | 1.00 | 36.56 |
| ATOM | 3200 | O   | HIS | 507 | 65.407 | 45.670 | 100.173 | 1.00 | 38.46 |
| ATOM | 3201 | N   | SER | 508 | 67.458 | 45.227 | 99.372  | 1.00 | 36.54 |
| ATOM | 3202 | CA  | SER | 508 | 68.083 | 46.427 | 99.917  | 1.00 | 36.63 |
| ATOM | 3203 | CB  | SER | 508 | 68.229 | 46.328 | 101.438 | 1.00 | 37.89 |
| ATOM | 3204 | OG  | SER | 508 | 69.053 | 45.232 | 101.811 | 1.00 | 39.59 |
| ATOM | 3205 | C   | SER | 508 | 69.458 | 46.530 | 99.296  | 1.00 | 36.63 |
| ATOM | 3206 | O   | SER | 508 | 69.994 | 45.527 | 98.824  | 1.00 | 36.76 |
| ATOM | 3207 | N   | TYR | 509 | 70.012 | 47.738 | 99.274  | 1.00 | 37.19 |
| ATOM | 3208 | CA  | TYR | 509 | 71.346 | 47.968 | 98.727  | 1.00 | 39.23 |
| ATOM | 3209 | CB  | TYR | 509 | 71.360 | 47.768 | 97.208  | 1.00 | 33.64 |
| ATOM | 3210 | CG  | TYR | 509 | 70.764 | 48.911 | 96.415  | 1.00 | 29.36 |
| ATOM | 3211 | CD1 | TYR | 509 | 71.578 | 49.902 | 95.870  | 1.00 | 27.11 |
| ATOM | 3212 | CE1 | TYR | 509 | 71.046 | 50.942 | 95.118  | 1.00 | 22.91 |
| ATOM | 3213 | CD2 | TYR | 509 | 69.392 | 48.990 | 96.189  | 1.00 | 26.29 |
| ATOM | 3214 | CE2 | TYR | 509 | 68.849 | 50.027 | 95.437  | 1.00 | 25.07 |
| ATOM | 3215 | CZ  | TYR | 509 | 69.683 | 50.999 | 94.902  | 1.00 | 23.09 |
| ATOM | 3216 | OH  | TYR | 509 | 69.155 | 52.024 | 94.146  | 1.00 | 24.38 |
| ATOM | 3217 | C   | TYR | 509 | 71.835 | 49.374 | 99.048  | 1.00 | 42.36 |
| ATOM | 3218 | O   | TYR | 509 | 71.051 | 50.252 | 99.404  | 1.00 | 43.20 |
| ATOM | 3219 | N   | GLU | 510 | 73.138 | 49.574 | 98.930  | 1.00 | 46.38 |
| ATOM | 3220 | CA  | GLU | 510 | 73.746 | 50.873 | 99.159  | 1.00 | 50.81 |
| ATOM | 3221 | CB  | GLU | 510 | 74.723 | 50.813 | 100.334 | 1.00 | 53.83 |
| ATOM | 3222 | CG  | GLU | 510 | 75.845 | 49.801 | 100.161 | 1.00 | 63.78 |
| ATOM | 3223 | CD  | GLU | 510 | 76.718 | 49.675 | 101.394 | 1.00 | 71.79 |
| ATOM | 3224 | OE1 | GLU | 510 | 76.330 | 48.919 | 102.314 | 1.00 | 75.41 |
| ATOM | 3225 | OE2 | GLU | 510 | 77.788 | 50.325 | 101.441 | 1.00 | 73.41 |
| ATOM | 3226 | C   | GLU | 510 | 74.482 | 51.166 | 97.857  | 1.00 | 52.99 |
| ATOM | 3227 | O   | GLU | 510 | 74.884 | 50.238 | 97.148  | 1.00 | 53.50 |
| ATOM | 3228 | N   | LYS | 511 | 74.621 | 52.439 | 97.509  | 1.00 | 54.97 |
| ATOM | 3229 | CA  | LYS | 511 | 75.312 | 52.795 | 96.280  | 1.00 | 55.10 |
| ATOM | 3230 | CB  | LYS | 511 | 74.354 | 53.494 | 95.312  | 1.00 | 56.27 |
| ATOM | 3231 | CG  | LYS | 511 | 74.918 | 53.698 | 93.908  | 1.00 | 57.13 |
| ATOM | 3232 | CD  | LYS | 511 | 73.909 | 54.392 | 92.994  | 1.00 | 58.18 |
| ATOM | 3233 | CE  | LYS | 511 | 72.631 | 53.576 | 92.849  | 1.00 | 59.33 |
| ATOM | 3234 | NZ  | LYS | 511 | 71.639 | 54.229 | 91.955  | 1.00 | 58.37 |
| ATOM | 3235 | C   | LYS | 511 | 76.507 | 53.688 | 96.571  | 1.00 | 54.99 |
| ATOM | 3236 | O   | LYS | 511 | 76.424 | 54.609 | 97.382  | 1.00 | 54.53 |
| ATOM | 3237 | N   | ARG | 512 | 77.628 | 53.362 | 95.942  | 1.00 | 56.46 |
| ATOM | 3238 | CA  | ARG | 512 | 78.868 | 54.115 | 96.081  | 1.00 | 57.97 |
| ATOM | 3239 | CB  | ARG | 512 | 79.803 | 53.447 | 97.085  | 1.00 | 58.04 |
| ATOM | 3240 | CG  | ARG | 512 | 79.468 | 53.766 | 98.529  | 1.00 | 62.49 |
| ATOM | 3241 | CD  | ARG | 512 | 80.493 | 53.185 | 99.482  | 1.00 | 64.62 |
| ATOM | 3242 | NE  | ARG | 512 | 80.419 | 51.727 | 99.537  | 1.00 | 63.61 |
| ATOM | 3243 | CZ  | ARG | 512 | 81.447 | 50.933 | 99.823  | 1.00 | 61.12 |
| ATOM | 3244 | NH1 | ARG | 512 | 82.644 | 51.445 | 100.083 | 1.00 | 56.55 |
| ATOM | 3245 | NH2 | ARG | 512 | 81.269 | 49.621 | 99.853  | 1.00 | 61.94 |



FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3246 | C   | ARG | 512  | 79.500 | 54.115 | 94.702 | 1.00 | 58.54 |
| ATOM | 3247 | O   | ARG | 512  | 79.178 | 53.252 | 93.884 | 1.00 | 59.96 |
| ATOM | 3248 | N   | LEU | 513  | 80.391 | 55.065 | 94.434 | 1.00 | 57.83 |
| ATOM | 3249 | CA  | LEU | 513  | 81.016 | 55.124 | 93.123 | 1.00 | 57.56 |
| ATOM | 3250 | CB  | LEU | 513  | 80.303 | 56.148 | 92.257 | 1.00 | 61.92 |
| ATOM | 3251 | CG  | LEU | 513  | 79.439 | 55.464 | 91.197 | 1.00 | 68.38 |
| ATOM | 3252 | CD1 | LEU | 513  | 78.247 | 56.348 | 90.818 | 1.00 | 71.78 |
| ATOM | 3253 | CD2 | LEU | 513  | 80.308 | 55.085 | 89.991 | 1.00 | 65.83 |
| ATOM | 3254 | C   | LEU | 513  | 82.510 | 55.358 | 93.107 | 1.00 | 55.65 |
| ATOM | 3255 | O   | LEU | 513  | 83.188 | 54.979 | 92.152 | 1.00 | 55.17 |
| ATOM | 3256 | N   | PHE | 514  | 83.012 | 55.993 | 94.157 | 1.00 | 54.01 |
| ATOM | 3257 | CA  | PHE | 514  | 84.434 | 56.272 | 94.282 | 1.00 | 52.79 |
| ATOM | 3258 | CB  | PHE | 514  | 84.809 | 57.567 | 93.540 | 1.00 | 51.46 |
| ATOM | 3259 | CG  | PHE | 514  | 84.134 | 58.813 | 94.071 | 1.00 | 47.21 |
| ATOM | 3260 | CD1 | PHE | 514  | 82.819 | 59.113 | 93.731 | 1.00 | 45.39 |
| ATOM | 3261 | CD2 | PHE | 514  | 84.833 | 59.707 | 94.873 | 1.00 | 42.42 |
| ATOM | 3262 | CE1 | PHE | 514  | 82.217 | 60.281 | 94.180 | 1.00 | 44.25 |
| ATOM | 3263 | CE2 | PHE | 514  | 84.238 | 60.874 | 95.325 | 1.00 | 41.86 |
| ATOM | 3264 | CZ  | PHE | 514  | 82.930 | 61.163 | 94.978 | 1.00 | 43.49 |
| ATOM | 3265 | C   | PHE | 514  | 84.837 | 56.352 | 95.752 | 1.00 | 52.80 |
| ATOM | 3266 | O   | PHE | 514  | 83.988 | 55.991 | 96.597 | 1.00 | 52.32 |
| ATOM | 3267 | CB  | SER | 1011 | 57.929 | 87.366 | 59.237 | 1.00 | 58.03 |
| ATOM | 3268 | OG  | SER | 1011 | 58.006 | 88.780 | 59.293 | 1.00 | 63.01 |
| ATOM | 3269 | C   | SER | 1011 | 59.129 | 85.247 | 59.802 | 1.00 | 54.25 |
| ATOM | 3270 | O   | SER | 1011 | 60.185 | 84.781 | 59.351 | 1.00 | 53.59 |
| ATOM | 3271 | N   | SER | 1011 | 60.325 | 87.376 | 59.863 | 1.00 | 55.40 |
| ATOM | 3272 | CA  | SER | 1011 | 59.010 | 86.732 | 60.117 | 1.00 | 55.46 |
| ATOM | 3273 | N   | TYR | 1012 | 58.046 | 84.513 | 60.043 | 1.00 | 51.61 |
| ATOM | 3274 | CA  | TYR | 1012 | 58.026 | 83.086 | 59.791 | 1.00 | 48.08 |
| ATOM | 3275 | CB  | TYR | 1012 | 56.873 | 82.419 | 60.545 | 1.00 | 41.27 |
| ATOM | 3276 | CG  | TYR | 1012 | 56.809 | 80.925 | 60.332 | 1.00 | 34.35 |
| ATOM | 3277 | CD1 | TYR | 1012 | 57.930 | 80.127 | 60.548 | 1.00 | 28.76 |
| ATOM | 3278 | CE1 | TYR | 1012 | 57.899 | 78.760 | 60.325 | 1.00 | 29.64 |
| ATOM | 3279 | CD2 | TYR | 1012 | 55.641 | 80.312 | 59.888 | 1.00 | 34.30 |
| ATOM | 3280 | CE2 | TYR | 1012 | 55.597 | 78.934 | 59.663 | 1.00 | 36.50 |
| ATOM | 3281 | CZ  | TYR | 1012 | 56.734 | 78.163 | 59.885 | 1.00 | 34.98 |
| ATOM | 3282 | OH  | TYR | 1012 | 56.704 | 76.797 | 59.672 | 1.00 | 36.25 |
| ATOM | 3283 | C   | TYR | 1012 | 57.892 | 82.790 | 58.309 | 1.00 | 48.56 |
| ATOM | 3284 | O   | TYR | 1012 | 57.098 | 83.422 | 57.604 | 1.00 | 49.57 |
| ATOM | 3285 | N   | VAL | 1013 | 58.707 | 81.859 | 57.833 | 1.00 | 48.25 |
| ATOM | 3286 | CA  | VAL | 1013 | 58.651 | 81.436 | 56.446 | 1.00 | 47.55 |
| ATOM | 3287 | CB  | VAL | 1013 | 59.816 | 81.975 | 55.598 | 1.00 | 48.39 |
| ATOM | 3288 | CG1 | VAL | 1013 | 59.361 | 82.123 | 54.154 | 1.00 | 47.70 |
| ATOM | 3289 | CG2 | VAL | 1013 | 60.348 | 83.289 | 56.162 | 1.00 | 49.99 |
| ATOM | 3290 | C   | VAL | 1013 | 58.732 | 79.916 | 56.490 | 1.00 | 47.43 |
| ATOM | 3291 | O   | VAL | 1013 | 59.714 | 79.348 | 56.978 | 1.00 | 47.21 |
| ATOM | 3292 | N   | PRO | 1014 | 57.640 | 79.243 | 56.114 | 1.00 | 47.63 |
| ATOM | 3293 | CD  | PRO | 1014 | 56.292 | 79.787 | 55.872 | 1.00 | 47.66 |
| ATOM | 3294 | CA  | PRO | 1014 | 57.622 | 77.781 | 56.122 | 1.00 | 48.55 |
| ATOM | 3295 | CB  | PRO | 1014 | 56.148 | 77.452 | 55.855 | 1.00 | 49.13 |
| ATOM | 3296 | CG  | PRO | 1014 | 55.629 | 78.665 | 55.137 | 1.00 | 49.10 |
| ATOM | 3297 | C   | PRO | 1014 | 58.568 | 77.153 | 55.097 | 1.00 | 48.71 |
| ATOM | 3298 | O   | PRO | 1014 | 58.646 | 77.595 | 53.944 | 1.00 | 49.40 |
| ATOM | 3299 | N   | ASP | 1015 | 59.323 | 76.153 | 55.549 | 1.00 | 48.60 |
| ATOM | 3300 | CA  | ASP | 1015 | 60.273 | 75.454 | 54.687 | 1.00 | 48.10 |
| ATOM | 3301 | CB  | ASP | 1015 | 61.138 | 74.468 | 55.501 | 1.00 | 53.10 |
| ATOM | 3302 | CG  | ASP | 1015 | 60.310 | 73.484 | 56.334 | 1.00 | 60.22 |
| ATOM | 3303 | OD1 | ASP | 1015 | 59.891 | 73.846 | 57.460 | 1.00 | 63.12 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3304 | OD2 | ASP | 1015 | 60.104 | 72.338 | 55.873 | 1.00 | 64.06 |
| ATOM | 3305 | C   | ASP | 1015 | 59.552 | 74.750 | 53.538 | 1.00 | 44.68 |
| ATOM | 3306 | O   | ASP | 1015 | 58.389 | 74.360 | 53.659 | 1.00 | 44.03 |
| ATOM | 3307 | N   | ASP | 1016 | 60.250 | 74.583 | 52.425 | 1.00 | 40.80 |
| ATOM | 3308 | CA  | ASP | 1016 | 59.657 | 73.952 | 51.264 | 1.00 | 38.03 |
| ATOM | 3309 | CB  | ASP | 1016 | 59.204 | 75.037 | 50.278 | 1.00 | 39.43 |
| ATOM | 3310 | CG  | ASP | 1016 | 57.769 | 74.858 | 49.822 | 1.00 | 38.43 |
| ATOM | 3311 | OD1 | ASP | 1016 | 57.008 | 75.848 | 49.852 | 1.00 | 34.54 |
| ATOM | 3312 | OD2 | ASP | 1016 | 57.405 | 73.730 | 49.430 | 1.00 | 41.54 |
| ATOM | 3313 | C   | ASP | 1016 | 60.665 | 73.024 | 50.594 | 1.00 | 35.83 |
| ATOM | 3314 | O   | ASP | 1016 | 61.813 | 73.399 | 50.366 | 1.00 | 37.51 |
| ATOM | 3315 | N   | GLY | 1017 | 60.230 | 71.811 | 50.285 | 1.00 | 32.24 |
| ATOM | 3316 | CA  | GLY | 1017 | 61.101 | 70.858 | 49.630 | 1.00 | 27.23 |
| ATOM | 3317 | C   | GLY | 1017 | 61.868 | 69.973 | 50.589 | 1.00 | 25.42 |
| ATOM | 3318 | O   | GLY | 1017 | 61.837 | 70.165 | 51.804 | 1.00 | 27.96 |
| ATOM | 3319 | N   | LEU | 1018 | 62.552 | 68.985 | 50.029 | 1.00 | 22.02 |
| ATOM | 3320 | CA  | LEU | 1018 | 63.340 | 68.043 | 50.798 | 1.00 | 18.75 |
| ATOM | 3321 | CB  | LEU | 1018 | 63.108 | 66.632 | 50.268 | 1.00 | 17.25 |
| ATOM | 3322 | CG  | LEU | 1018 | 61.713 | 66.062 | 50.485 | 1.00 | 16.23 |
| ATOM | 3323 | CD1 | LEU | 1018 | 61.601 | 64.734 | 49.768 | 1.00 | 16.81 |
| ATOM | 3324 | CD2 | LEU | 1018 | 61.452 | 65.896 | 51.978 | 1.00 | 13.24 |
| ATOM | 3325 | C   | LEU | 1018 | 64.814 | 68.361 | 50.687 | 1.00 | 15.88 |
| ATOM | 3326 | O   | LEU | 1018 | 65.252 | 68.972 | 49.724 | 1.00 | 17.36 |
| ATOM | 3327 | N   | THR | 1019 | 65.580 | 67.966 | 51.687 | 1.00 | 13.27 |
| ATOM | 3328 | CA  | THR | 1019 | 67.007 | 68.179 | 51.634 | 1.00 | 14.14 |
| ATOM | 3329 | CB  | THR | 1019 | 67.611 | 68.222 | 53.031 | 1.00 | 12.51 |
| ATOM | 3330 | OG1 | THR | 1019 | 67.263 | 67.029 | 53.737 | 1.00 | 17.30 |
| ATOM | 3331 | CG2 | THR | 1019 | 67.076 | 69.419 | 53.799 | 1.00 | 8.68  |
| ATOM | 3332 | C   | THR | 1019 | 67.505 | 66.954 | 50.878 | 1.00 | 16.62 |
| ATOM | 3333 | O   | THR | 1019 | 66.768 | 65.967 | 50.761 | 1.00 | 17.81 |
| ATOM | 3334 | N   | ALA | 1020 | 68.723 | 67.007 | 50.341 | 1.00 | 16.80 |
| ATOM | 3335 | CA  | ALA | 1020 | 69.253 | 65.872 | 49.598 | 1.00 | 16.84 |
| ATOM | 3336 | CB  | ALA | 1020 | 70.620 | 66.183 | 49.042 | 1.00 | 17.48 |
| ATOM | 3337 | C   | ALA | 1020 | 69.282 | 64.630 | 50.485 | 1.00 | 17.70 |
| ATOM | 3338 | O   | ALA | 1020 | 69.021 | 63.514 | 50.020 | 1.00 | 19.09 |
| ATOM | 3339 | N   | GLN | 1021 | 69.548 | 64.825 | 51.771 | 1.00 | 16.33 |
| ATOM | 3340 | CA  | GLN | 1021 | 69.568 | 63.704 | 52.693 | 1.00 | 17.71 |
| ATOM | 3341 | CB  | GLN | 1021 | 70.003 | 64.152 | 54.088 | 1.00 | 21.58 |
| ATOM | 3342 | CG  | GLN | 1021 | 69.993 | 63.035 | 55.126 | 1.00 | 33.97 |
| ATOM | 3343 | CD  | GLN | 1021 | 71.118 | 63.171 | 56.141 | 1.00 | 44.79 |
| ATOM | 3344 | OE1 | GLN | 1021 | 71.121 | 64.087 | 56.972 | 1.00 | 47.71 |
| ATOM | 3345 | NE2 | GLN | 1021 | 72.092 | 62.267 | 56.068 | 1.00 | 49.18 |
| ATOM | 3346 | C   | GLN | 1021 | 68.202 | 63.012 | 52.754 | 1.00 | 17.20 |
| ATOM | 3347 | O   | GLN | 1021 | 68.118 | 61.805 | 52.578 | 1.00 | 17.20 |
| ATOM | 3348 | N   | GLN | 1022 | 67.131 | 63.778 | 52.944 | 1.00 | 16.52 |
| ATOM | 3349 | CA  | GLN | 1022 | 65.790 | 63.202 | 53.028 | 1.00 | 15.89 |
| ATOM | 3350 | CB  | GLN | 1022 | 64.758 | 64.276 | 53.323 | 1.00 | 15.47 |
| ATOM | 3351 | CG  | GLN | 1022 | 65.023 | 65.126 | 54.536 | 1.00 | 17.25 |
| ATOM | 3352 | CD  | GLN | 1022 | 63.960 | 66.191 | 54.684 | 1.00 | 23.78 |
| ATOM | 3353 | OE1 | GLN | 1022 | 62.816 | 65.890 | 55.009 | 1.00 | 31.89 |
| ATOM | 3354 | NE2 | GLN | 1022 | 64.318 | 67.436 | 54.403 | 1.00 | 26.89 |
| ATOM | 3355 | C   | GLN | 1022 | 65.381 | 62.524 | 51.733 | 1.00 | 17.02 |
| ATOM | 3356 | O   | GLN | 1022 | 64.887 | 61.402 | 51.731 | 1.00 | 19.29 |
| ATOM | 3357 | N   | LEU | 1023 | 65.579 | 63.237 | 50.635 | 1.00 | 17.87 |
| ATOM | 3358 | CA  | LEU | 1023 | 65.228 | 62.773 | 49.307 | 1.00 | 17.81 |
| ATOM | 3359 | CB  | LEU | 1023 | 65.552 | 63.877 | 48.291 | 1.00 | 18.45 |
| ATOM | 3360 | CG  | LEU | 1023 | 65.210 | 63.689 | 46.812 | 1.00 | 19.08 |
| ATOM | 3361 | CD1 | LEU | 1023 | 63.703 | 63.664 | 46.612 | 1.00 | 18.39 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3362 | CD2 | LEU | 1023 | 65.827 | 64.815 | 46.014 | 1.00 | 16.88 |
| ATOM | 3363 | C   | LEU | 1023 | 65.927 | 61.479 | 48.909 | 1.00 | 20.42 |
| ATOM | 3364 | O   | LEU | 1023 | 65.280 | 60.543 | 48.436 | 1.00 | 19.06 |
| ATOM | 3365 | N   | PHE | 1024 | 67.244 | 61.425 | 49.093 | 1.00 | 23.89 |
| ATOM | 3366 | CA  | PHE | 1024 | 68.023 | 60.249 | 48.704 | 1.00 | 25.50 |
| ATOM | 3367 | CB  | PHE | 1024 | 69.421 | 60.657 | 48.257 | 1.00 | 19.33 |
| ATOM | 3368 | CG  | PHE | 1024 | 69.405 | 61.431 | 46.990 | 1.00 | 17.62 |
| ATOM | 3369 | CD1 | PHE | 1024 | 69.404 | 60.778 | 45.770 | 1.00 | 16.25 |
| ATOM | 3370 | CD2 | PHE | 1024 | 69.241 | 62.810 | 47.013 | 1.00 | 23.98 |
| ATOM | 3371 | CE1 | PHE | 1024 | 69.226 | 61.477 | 44.590 | 1.00 | 21.25 |
| ATOM | 3372 | CE2 | PHE | 1024 | 69.062 | 63.525 | 45.841 | 1.00 | 25.54 |
| ATOM | 3373 | CZ  | PHE | 1024 | 69.052 | 62.856 | 44.625 | 1.00 | 27.04 |
| ATOM | 3374 | C   | PHE | 1024 | 68.064 | 59.117 | 49.693 | 1.00 | 28.39 |
| ATOM | 3375 | O   | PHE | 1024 | 68.248 | 57.961 | 49.321 | 1.00 | 30.05 |
| ATOM | 3376 | N   | ASN | 1025 | 67.867 | 59.444 | 50.957 | 1.00 | 31.89 |
| ATOM | 3377 | CA  | ASN | 1025 | 67.846 | 58.427 | 51.987 | 1.00 | 36.32 |
| ATOM | 3378 | CB  | ASN | 1025 | 68.597 | 58.917 | 53.232 | 1.00 | 41.18 |
| ATOM | 3379 | CG  | ASN | 1025 | 70.085 | 59.192 | 52.944 | 1.00 | 41.83 |
| ATOM | 3380 | OD1 | ASN | 1025 | 70.957 | 58.409 | 53.319 | 1.00 | 47.33 |
| ATOM | 3381 | ND2 | ASN | 1025 | 70.369 | 60.292 | 52.263 | 1.00 | 38.75 |
| ATOM | 3382 | C   | ASN | 1025 | 66.357 | 58.169 | 52.207 | 1.00 | 36.28 |
| ATOM | 3383 | O   | ASN | 1025 | 65.818 | 58.279 | 53.313 | 1.00 | 36.13 |
| ATOM | 3384 | N   | CYS | 1026 | 65.724 | 57.839 | 51.080 | 1.00 | 36.85 |
| ATOM | 3385 | CA  | CYS | 1026 | 64.298 | 57.551 | 50.945 | 1.00 | 34.82 |
| ATOM | 3386 | CB  | CYS | 1026 | 63.662 | 58.629 | 50.061 | 1.00 | 37.24 |
| ATOM | 3387 | SG  | CYS | 1026 | 62.051 | 59.254 | 50.560 | 1.00 | 47.39 |
| ATOM | 3388 | C   | CYS | 1026 | 64.120 | 56.177 | 50.266 | 1.00 | 33.53 |
| ATOM | 3389 | O   | CYS | 1026 | 63.007 | 55.667 | 50.174 | 1.00 | 32.71 |
| ATOM | 3390 | N   | GLY | 1027 | 65.204 | 55.624 | 49.723 | 1.00 | 32.56 |
| ATOM | 3391 | CA  | GLY | 1027 | 65.154 | 54.316 | 49.082 | 1.00 | 31.56 |
| ATOM | 3392 | C   | GLY | 1027 | 64.429 | 54.193 | 47.749 | 1.00 | 31.84 |
| ATOM | 3393 | O   | GLY | 1027 | 64.181 | 53.084 | 47.270 | 1.00 | 30.93 |
| ATOM | 3394 | N   | ASP | 1028 | 64.141 | 55.323 | 47.119 | 1.00 | 31.14 |
| ATOM | 3395 | CA  | ASP | 1028 | 63.421 | 55.326 | 45.853 | 1.00 | 30.56 |
| ATOM | 3396 | CB  | ASP | 1028 | 62.755 | 56.691 | 45.623 | 1.00 | 36.90 |
| ATOM | 3397 | CG  | ASP | 1028 | 61.541 | 56.924 | 46.530 | 1.00 | 43.07 |
| ATOM | 3398 | OD1 | ASP | 1028 | 60.926 | 55.938 | 47.010 | 1.00 | 45.77 |
| ATOM | 3399 | OD2 | ASP | 1028 | 61.193 | 58.108 | 46.742 | 1.00 | 46.97 |
| ATOM | 3400 | C   | ASP | 1028 | 64.230 | 54.935 | 44.622 | 1.00 | 28.09 |
| ATOM | 3401 | O   | ASP | 1028 | 63.652 | 54.695 | 43.563 | 1.00 | 28.66 |
| ATOM | 3402 | N   | GLY | 1029 | 65.553 | 54.898 | 44.744 | 1.00 | 24.86 |
| ATOM | 3403 | CA  | GLY | 1029 | 66.378 | 54.534 | 43.606 | 1.00 | 21.35 |
| ATOM | 3404 | C   | GLY | 1029 | 66.189 | 55.526 | 42.471 | 1.00 | 21.27 |
| ATOM | 3405 | O   | GLY | 1029 | 65.868 | 55.145 | 41.332 | 1.00 | 21.10 |
| ATOM | 3406 | N   | LEU | 1030 | 66.397 | 56.806 | 42.774 | 1.00 | 20.08 |
| ATOM | 3407 | CA  | LEU | 1030 | 66.225 | 57.848 | 41.772 | 1.00 | 18.05 |
| ATOM | 3408 | CB  | LEU | 1030 | 65.340 | 58.992 | 42.303 | 1.00 | 17.70 |
| ATOM | 3409 | CG  | LEU | 1030 | 65.138 | 59.328 | 43.782 | 1.00 | 14.68 |
| ATOM | 3410 | CD1 | LEU | 1030 | 66.426 | 59.721 | 44.418 | 1.00 | 21.75 |
| ATOM | 3411 | CD2 | LEU | 1030 | 64.175 | 60.474 | 43.905 | 1.00 | 13.20 |
| ATOM | 3412 | C   | LEU | 1030 | 67.490 | 58.408 | 41.126 | 1.00 | 18.04 |
| ATOM | 3413 | O   | LEU | 1030 | 68.601 | 58.272 | 41.651 | 1.00 | 15.80 |
| ATOM | 3414 | N   | THR | 1031 | 67.303 | 58.964 | 39.932 | 1.00 | 18.36 |
| ATOM | 3415 | CA  | THR | 1031 | 68.371 | 59.591 | 39.167 | 1.00 | 17.66 |
| ATOM | 3416 | CB  | THR | 1031 | 68.653 | 58.880 | 37.850 | 1.00 | 17.35 |
| ATOM | 3417 | OG1 | THR | 1031 | 67.489 | 58.168 | 37.410 | 1.00 | 20.68 |
| ATOM | 3418 | CG2 | THR | 1031 | 69.798 | 57.957 | 38.023 | 1.00 | 19.52 |
| ATOM | 3419 | C   | THR | 1031 | 68.014 | 61.024 | 38.850 | 1.00 | 17.30 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3420 | O   | THR | 1031 | 66.990 | 61.528 | 39.295 | 1.00 | 18.68 |
| ATOM | 3421 | N   | TYR | 1032 | 68.834 | 61.641 | 38.012 | 1.00 | 16.44 |
| ATOM | 3422 | CA  | TYR | 1032 | 68.674 | 63.031 | 37.617 | 1.00 | 16.87 |
| ATOM | 3423 | CB  | TYR | 1032 | 69.631 | 63.343 | 36.463 | 1.00 | 14.97 |
| ATOM | 3424 | CG  | TYR | 1032 | 71.073 | 63.021 | 36.756 | 1.00 | 8.96  |
| ATOM | 3425 | CD1 | TYR | 1032 | 71.641 | 63.357 | 37.975 | 1.00 | 11.80 |
| ATOM | 3426 | CE1 | TYR | 1032 | 72.972 | 63.071 | 38.250 | 1.00 | 14.63 |
| ATOM | 3427 | CD2 | TYR | 1032 | 71.870 | 62.390 | 35.809 | 1.00 | 5.18  |
| ATOM | 3428 | CE2 | TYR | 1032 | 73.194 | 62.102 | 36.068 | 1.00 | 7.16  |
| ATOM | 3429 | CZ  | TYR | 1032 | 73.746 | 62.447 | 37.291 | 1.00 | 12.40 |
| ATOM | 3430 | OH  | TYR | 1032 | 75.074 | 62.186 | 37.557 | 1.00 | 13.92 |
| ATOM | 3431 | C   | TYR | 1032 | 67.266 | 63.513 | 37.249 | 1.00 | 18.29 |
| ATOM | 3432 | O   | TYR | 1032 | 66.758 | 64.472 | 37.834 | 1.00 | 16.95 |
| ATOM | 3433 | N   | ASN | 1033 | 66.623 | 62.840 | 36.301 | 1.00 | 19.44 |
| ATOM | 3434 | CA  | ASN | 1033 | 65.304 | 63.277 | 35.860 | 1.00 | 19.44 |
| ATOM | 3435 | CB  | ASN | 1033 | 64.954 | 62.644 | 34.519 | 1.00 | 17.51 |
| ATOM | 3436 | CG  | ASN | 1033 | 65.762 | 63.226 | 33.386 | 1.00 | 24.27 |
| ATOM | 3437 | OD1 | ASN | 1033 | 66.375 | 64.288 | 33.528 | 1.00 | 27.27 |
| ATOM | 3438 | ND2 | ASN | 1033 | 65.795 | 62.530 | 32.261 | 1.00 | 24.84 |
| ATOM | 3439 | C   | ASN | 1033 | 64.154 | 63.126 | 36.833 | 1.00 | 19.96 |
| ATOM | 3440 | O   | ASN | 1033 | 63.058 | 63.613 | 36.570 | 1.00 | 21.81 |
| ATOM | 3441 | N   | ASP | 1034 | 64.413 | 62.507 | 37.977 | 1.00 | 18.51 |
| ATOM | 3442 | CA  | ASP | 1034 | 63.369 | 62.288 | 38.966 | 1.00 | 16.08 |
| ATOM | 3443 | CB  | ASP | 1034 | 63.602 | 60.964 | 39.695 | 1.00 | 13.85 |
| ATOM | 3444 | CG  | ASP | 1034 | 63.376 | 59.770 | 38.806 | 1.00 | 17.69 |
| ATOM | 3445 | OD1 | ASP | 1034 | 62.332 | 59.729 | 38.121 | 1.00 | 22.84 |
| ATOM | 3446 | OD2 | ASP | 1034 | 64.242 | 58.877 | 38.783 | 1.00 | 17.41 |
| ATOM | 3447 | C   | ASP | 1034 | 63.212 | 63.402 | 39.979 | 1.00 | 15.01 |
| ATOM | 3448 | O   | ASP | 1034 | 62.325 | 63.326 | 40.835 | 1.00 | 17.19 |
| ATOM | 3449 | N   | PHE | 1035 | 64.053 | 64.426 | 39.910 | 1.00 | 11.94 |
| ATOM | 3450 | CA  | PHE | 1035 | 63.942 | 65.504 | 40.881 | 1.00 | 12.57 |
| ATOM | 3451 | CB  | PHE | 1035 | 64.743 | 65.178 | 42.149 | 1.00 | 10.75 |
| ATOM | 3452 | CG  | PHE | 1035 | 66.224 | 65.195 | 41.946 | 1.00 | 10.13 |
| ATOM | 3453 | CD1 | PHE | 1035 | 66.943 | 66.375 | 42.108 | 1.00 | 12.40 |
| ATOM | 3454 | CD2 | PHE | 1035 | 66.897 | 64.044 | 41.572 | 1.00 | 13.01 |
| ATOM | 3455 | CE1 | PHE | 1035 | 68.315 | 66.405 | 41.901 | 1.00 | 14.59 |
| ATOM | 3456 | CE2 | PHE | 1035 | 68.275 | 64.059 | 41.361 | 1.00 | 17.26 |
| ATOM | 3457 | CZ  | PHE | 1035 | 68.986 | 65.241 | 41.524 | 1.00 | 16.88 |
| ATOM | 3458 | C   | PHE | 1035 | 64.344 | 66.866 | 40.345 | 1.00 | 12.04 |
| ATOM | 3459 | O   | PHE | 1035 | 64.903 | 66.984 | 39.257 | 1.00 | 11.35 |
| ATOM | 3460 | N   | LEU | 1036 | 64.061 | 67.889 | 41.138 | 1.00 | 12.75 |
| ATOM | 3461 | CA  | LEU | 1036 | 64.372 | 69.261 | 40.774 | 1.00 | 16.81 |
| ATOM | 3462 | CB  | LEU | 1036 | 63.098 | 69.993 | 40.359 | 1.00 | 17.81 |
| ATOM | 3463 | CG  | LEU | 1036 | 62.568 | 69.755 | 38.955 | 1.00 | 18.45 |
| ATOM | 3464 | CD1 | LEU | 1036 | 61.203 | 70.408 | 38.829 | 1.00 | 15.39 |
| ATOM | 3465 | CD2 | LEU | 1036 | 63.555 | 70.308 | 37.936 | 1.00 | 18.87 |
| ATOM | 3466 | C   | LEU | 1036 | 64.992 | 70.009 | 41.941 | 1.00 | 17.35 |
| ATOM | 3467 | O   | LEU | 1036 | 64.808 | 69.633 | 43.100 | 1.00 | 20.23 |
| ATOM | 3468 | N   | ILE | 1037 | 65.745 | 71.056 | 41.626 | 1.00 | 15.55 |
| ATOM | 3469 | CA  | ILE | 1037 | 66.354 | 71.878 | 42.648 | 1.00 | 12.98 |
| ATOM | 3470 | CB  | ILE | 1037 | 67.771 | 72.312 | 42.254 | 1.00 | 13.94 |
| ATOM | 3471 | CG2 | ILE | 1037 | 68.491 | 72.873 | 43.470 | 1.00 | 13.02 |
| ATOM | 3472 | CG1 | ILE | 1037 | 68.555 | 71.115 | 41.698 | 1.00 | 16.53 |
| ATOM | 3473 | CD1 | ILE | 1037 | 69.945 | 71.454 | 41.180 | 1.00 | 13.78 |
| ATOM | 3474 | C   | ILE | 1037 | 65.445 | 73.095 | 42.706 | 1.00 | 13.09 |
| ATOM | 3475 | O   | ILE | 1037 | 65.202 | 73.744 | 41.680 | 1.00 | 13.21 |
| ATOM | 3476 | N   | LEU | 1038 | 64.861 | 73.344 | 43.869 | 1.00 | 10.11 |
| ATOM | 3477 | CA  | LEU | 1038 | 63.980 | 74.486 | 44.014 | 1.00 | 10.59 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3478 | CB  | LEU | 1038 | 63.183 | 74.398 | 45.322 | 1.00 | 10.09 |
| ATOM | 3479 | CG  | LEU | 1038 | 62.147 | 73.275 | 45.416 | 1.00 | 3.81  |
| ATOM | 3480 | CD1 | LEU | 1038 | 61.367 | 73.428 | 46.684 | 1.00 | 3.17  |
| ATOM | 3481 | CD2 | LEU | 1038 | 61.213 | 73.318 | 44.237 | 1.00 | 2.82  |
| ATOM | 3482 | C   | LEU | 1038 | 64.849 | 75.738 | 43.976 | 1.00 | 12.67 |
| ATOM | 3483 | O   | LEU | 1038 | 65.959 | 75.735 | 44.514 | 1.00 | 14.13 |
| ATOM | 3484 | N   | PRO | 1039 | 64.375 | 76.811 | 43.311 | 1.00 | 12.96 |
| ATOM | 3485 | CD  | PRO | 1039 | 63.052 | 76.923 | 42.671 | 1.00 | 13.41 |
| ATOM | 3486 | CA  | PRO | 1039 | 65.115 | 78.075 | 43.194 | 1.00 | 11.42 |
| ATOM | 3487 | CB  | PRO | 1039 | 64.226 | 78.890 | 42.262 | 1.00 | 12.86 |
| ATOM | 3488 | CG  | PRO | 1039 | 62.853 | 78.408 | 42.613 | 1.00 | 11.92 |
| ATOM | 3489 | C   | PRO | 1039 | 65.328 | 78.779 | 44.522 | 1.00 | 11.00 |
| ATOM | 3490 | O   | PRO | 1039 | 64.657 | 78.473 | 45.505 | 1.00 | 12.52 |
| ATOM | 3491 | N   | GLY | 1040 | 66.239 | 79.745 | 44.536 | 1.00 | 12.23 |
| ATOM | 3492 | CA  | GLY | 1040 | 66.525 | 80.482 | 45.754 | 1.00 | 12.18 |
| ATOM | 3493 | C   | GLY | 1040 | 66.517 | 81.987 | 45.570 | 1.00 | 12.14 |
| ATOM | 3494 | O   | GLY | 1040 | 65.700 | 82.516 | 44.821 | 1.00 | 13.21 |
| ATOM | 3495 | N   | TYR | 1041 | 67.434 | 82.671 | 46.248 | 1.00 | 13.56 |
| ATOM | 3496 | CA  | TYR | 1041 | 67.542 | 84.127 | 46.182 | 1.00 | 13.97 |
| ATOM | 3497 | CB  | TYR | 1041 | 67.703 | 84.702 | 47.593 | 1.00 | 14.19 |
| ATOM | 3498 | CG  | TYR | 1041 | 67.872 | 86.207 | 47.636 | 1.00 | 17.57 |
| ATOM | 3499 | CD1 | TYR | 1041 | 66.893 | 87.057 | 47.115 | 1.00 | 18.66 |
| ATOM | 3500 | CE1 | TYR | 1041 | 67.054 | 88.441 | 47.137 | 1.00 | 18.65 |
| ATOM | 3501 | CD2 | TYR | 1041 | 69.017 | 86.782 | 48.185 | 1.00 | 15.46 |
| ATOM | 3502 | CE2 | TYR | 1041 | 69.183 | 88.163 | 48.213 | 1.00 | 18.22 |
| ATOM | 3503 | CZ  | TYR | 1041 | 68.200 | 88.989 | 47.687 | 1.00 | 18.97 |
| ATOM | 3504 | OH  | TYR | 1041 | 68.374 | 90.361 | 47.714 | 1.00 | 19.15 |
| ATOM | 3505 | C   | TYR | 1041 | 68.720 | 84.550 | 45.313 | 1.00 | 14.59 |
| ATOM | 3506 | O   | TYR | 1041 | 69.868 | 84.240 | 45.631 | 1.00 | 16.29 |
| ATOM | 3507 | N   | ILE | 1042 | 68.434 | 85.272 | 44.231 | 1.00 | 15.26 |
| ATOM | 3508 | CA  | ILE | 1042 | 69.469 | 85.742 | 43.306 | 1.00 | 14.94 |
| ATOM | 3509 | CB  | ILE | 1042 | 68.926 | 85.844 | 41.871 | 1.00 | 11.71 |
| ATOM | 3510 | CG2 | ILE | 1042 | 70.016 | 86.310 | 40.926 | 1.00 | 7.14  |
| ATOM | 3511 | CG1 | ILE | 1042 | 68.367 | 84.483 | 41.444 | 1.00 | 8.36  |
| ATOM | 3512 | CD1 | ILE | 1042 | 67.843 | 84.452 | 40.058 | 1.00 | 5.40  |
| ATOM | 3513 | C   | ILE | 1042 | 70.068 | 87.074 | 43.744 | 1.00 | 17.59 |
| ATOM | 3514 | O   | ILE | 1042 | 69.428 | 88.127 | 43.688 | 1.00 | 18.42 |
| ATOM | 3515 | N   | ASP | 1043 | 71.331 | 87.011 | 44.130 | 1.00 | 21.17 |
| ATOM | 3516 | CA  | ASP | 1043 | 72.060 | 88.163 | 44.629 | 1.00 | 24.79 |
| ATOM | 3517 | CB  | ASP | 1043 | 72.676 | 87.773 | 45.978 | 1.00 | 25.19 |
| ATOM | 3518 | CG  | ASP | 1043 | 72.641 | 88.897 | 46.981 | 1.00 | 33.67 |
| ATOM | 3519 | OD1 | ASP | 1043 | 71.841 | 89.846 | 46.812 | 1.00 | 39.64 |
| ATOM | 3520 | OD2 | ASP | 1043 | 73.410 | 88.823 | 47.961 | 1.00 | 37.45 |
| ATOM | 3521 | C   | ASP | 1043 | 73.176 | 88.612 | 43.688 | 1.00 | 26.69 |
| ATOM | 3522 | O   | ASP | 1043 | 73.903 | 89.564 | 43.990 | 1.00 | 28.10 |
| ATOM | 3523 | N   | PHE | 1044 | 73.272 | 87.976 | 42.526 | 1.00 | 25.31 |
| ATOM | 3524 | CA  | PHE | 1044 | 74.343 | 88.271 | 41.587 | 1.00 | 22.89 |
| ATOM | 3525 | CB  | PHE | 1044 | 75.567 | 87.446 | 41.975 | 1.00 | 21.97 |
| ATOM | 3526 | CG  | PHE | 1044 | 75.286 | 85.977 | 42.022 | 1.00 | 25.11 |
| ATOM | 3527 | CD1 | PHE | 1044 | 74.503 | 85.440 | 43.048 | 1.00 | 24.61 |
| ATOM | 3528 | CD2 | PHE | 1044 | 75.696 | 85.145 | 40.991 | 1.00 | 25.66 |
| ATOM | 3529 | CE1 | PHE | 1044 | 74.127 | 84.108 | 43.034 | 1.00 | 22.42 |
| ATOM | 3530 | CE2 | PHE | 1044 | 75.321 | 83.806 | 40.972 | 1.00 | 24.74 |
| ATOM | 3531 | CZ  | PHE | 1044 | 74.535 | 83.291 | 41.994 | 1.00 | 23.97 |
| ATOM | 3532 | C   | PHE | 1044 | 73.946 | 87.861 | 40.186 | 1.00 | 23.67 |
| ATOM | 3533 | O   | PHE | 1044 | 72.930 | 87.193 | 39.974 | 1.00 | 24.13 |
| ATOM | 3534 | N   | THR | 1045 | 74.810 | 88.195 | 39.240 | 1.00 | 24.33 |
| ATOM | 3535 | CA  | THR | 1045 | 74.589 | 87.866 | 37.847 | 1.00 | 23.97 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3536 | CB  | THR | 1045 | 75.099 | 88.999 | 36.918 | 1.00 | 21.89 |
| ATOM | 3537 | OG1 | THR | 1045 | 76.524 | 89.071 | 36.965 | 1.00 | 22.39 |
| ATOM | 3538 | CG2 | THR | 1045 | 74.551 | 90.335 | 37.382 | 1.00 | 17.41 |
| ATOM | 3539 | C   | THR | 1045 | 75.307 | 86.552 | 37.558 | 1.00 | 24.74 |
| ATOM | 3540 | O   | THR | 1045 | 76.320 | 86.234 | 38.189 | 1.00 | 23.80 |
| ATOM | 3541 | N   | ALA | 1046 | 74.761 | 85.786 | 36.618 | 1.00 | 26.52 |
| ATOM | 3542 | CA  | ALA | 1046 | 75.305 | 84.487 | 36.229 | 1.00 | 26.11 |
| ATOM | 3543 | CB  | ALA | 1046 | 74.539 | 83.935 | 35.036 | 1.00 | 24.43 |
| ATOM | 3544 | C   | ALA | 1046 | 76.792 | 84.490 | 35.929 | 1.00 | 26.72 |
| ATOM | 3545 | O   | ALA | 1046 | 77.516 | 83.597 | 36.350 | 1.00 | 27.98 |
| ATOM | 3546 | N   | ASP | 1047 | 77.255 | 85.504 | 35.212 | 1.00 | 29.16 |
| ATOM | 3547 | CA  | ASP | 1047 | 78.666 | 85.586 | 34.851 | 1.00 | 31.33 |
| ATOM | 3548 | CB  | ASP | 1047 | 78.923 | 86.779 | 33.923 | 1.00 | 38.14 |
| ATOM | 3549 | CG  | ASP | 1047 | 78.465 | 88.107 | 34.519 | 1.00 | 46.25 |
| ATOM | 3550 | OD1 | ASP | 1047 | 79.291 | 88.799 | 35.165 | 1.00 | 48.68 |
| ATOM | 3551 | OD2 | ASP | 1047 | 77.279 | 88.467 | 34.319 | 1.00 | 50.20 |
| ATOM | 3552 | C   | ASP | 1047 | 79.604 | 85.638 | 36.046 | 1.00 | 28.88 |
| ATOM | 3553 | O   | ASP | 1047 | 80.810 | 85.557 | 35.890 | 1.00 | 31.35 |
| ATOM | 3554 | N   | GLN | 1048 | 79.049 | 85.740 | 37.241 | 1.00 | 27.79 |
| ATOM | 3555 | CA  | GLN | 1048 | 79.862 | 85.810 | 38.437 | 1.00 | 27.71 |
| ATOM | 3556 | CB  | GLN | 1048 | 79.237 | 86.797 | 39.411 | 1.00 | 31.21 |
| ATOM | 3557 | CG  | GLN | 1048 | 78.900 | 88.121 | 38.785 | 1.00 | 38.83 |
| ATOM | 3558 | CD  | GLN | 1048 | 78.268 | 89.067 | 39.771 | 1.00 | 47.10 |
| ATOM | 3559 | OE1 | GLN | 1048 | 77.175 | 89.582 | 39.547 | 1.00 | 49.42 |
| ATOM | 3560 | NE2 | GLN | 1048 | 78.953 | 89.305 | 40.879 | 1.00 | 52.51 |
| ATOM | 3561 | C   | GLN | 1048 | 80.025 | 84.471 | 39.133 | 1.00 | 26.49 |
| ATOM | 3562 | O   | GLN | 1048 | 80.688 | 84.393 | 40.165 | 1.00 | 29.30 |
| ATOM | 3563 | N   | VAL | 1049 | 79.406 | 83.427 | 38.598 | 1.00 | 23.74 |
| ATOM | 3564 | CA  | VAL | 1049 | 79.486 | 82.120 | 39.220 | 1.00 | 19.66 |
| ATOM | 3565 | CB  | VAL | 1049 | 78.365 | 81.196 | 38.736 | 1.00 | 19.77 |
| ATOM | 3566 | CG1 | VAL | 1049 | 78.453 | 79.838 | 39.437 | 1.00 | 14.56 |
| ATOM | 3567 | CG2 | VAL | 1049 | 77.014 | 81.850 | 39.003 | 1.00 | 21.34 |
| ATOM | 3568 | C   | VAL | 1049 | 80.820 | 81.478 | 38.945 | 1.00 | 19.62 |
| ATOM | 3569 | O   | VAL | 1049 | 81.276 | 81.442 | 37.810 | 1.00 | 22.57 |
| ATOM | 3570 | N   | ASP | 1050 | 81.437 | 80.964 | 39.998 | 1.00 | 18.17 |
| ATOM | 3571 | CA  | ASP | 1050 | 82.732 | 80.314 | 39.908 | 1.00 | 17.07 |
| ATOM | 3572 | CB  | ASP | 1050 | 83.546 | 80.635 | 41.163 | 1.00 | 16.95 |
| ATOM | 3573 | CG  | ASP | 1050 | 84.989 | 80.170 | 41.078 | 1.00 | 22.48 |
| ATOM | 3574 | OD1 | ASP | 1050 | 85.453 | 79.784 | 39.982 | 1.00 | 26.67 |
| ATOM | 3575 | OD2 | ASP | 1050 | 85.674 | 80.196 | 42.119 | 1.00 | 26.60 |
| ATOM | 3576 | C   | ASP | 1050 | 82.540 | 78.807 | 39.784 | 1.00 | 18.43 |
| ATOM | 3577 | O   | ASP | 1050 | 81.944 | 78.173 | 40.662 | 1.00 | 20.72 |
| ATOM | 3578 | N   | LEU | 1051 | 83.053 | 78.231 | 38.700 | 1.00 | 17.50 |
| ATOM | 3579 | CA  | LEU | 1051 | 82.944 | 76.792 | 38.483 | 1.00 | 14.50 |
| ATOM | 3580 | CB  | LEU | 1051 | 82.500 | 76.493 | 37.052 | 1.00 | 7.44  |
| ATOM | 3581 | CG  | LEU | 1051 | 81.227 | 77.157 | 36.539 | 1.00 | 5.31  |
| ATOM | 3582 | CD1 | LEU | 1051 | 80.887 | 76.556 | 35.188 | 1.00 | 4.75  |
| ATOM | 3583 | CD2 | LEU | 1051 | 80.076 | 76.967 | 37.519 | 1.00 | 3.50  |
| ATOM | 3584 | C   | LEU | 1051 | 84.244 | 76.035 | 38.768 | 1.00 | 15.17 |
| ATOM | 3585 | O   | LEU | 1051 | 84.392 | 74.894 | 38.344 | 1.00 | 14.20 |
| ATOM | 3586 | N   | THR | 1052 | 85.194 | 76.669 | 39.452 | 1.00 | 18.28 |
| ATOM | 3587 | CA  | THR | 1052 | 86.468 | 76.017 | 39.772 | 1.00 | 20.55 |
| ATOM | 3588 | CB  | THR | 1052 | 87.351 | 76.892 | 40.686 | 1.00 | 22.00 |
| ATOM | 3589 | OG1 | THR | 1052 | 87.488 | 78.202 | 40.115 | 1.00 | 16.85 |
| ATOM | 3590 | CG2 | THR | 1052 | 88.731 | 76.270 | 40.827 | 1.00 | 19.87 |
| ATOM | 3591 | C   | THR | 1052 | 86.172 | 74.698 | 40.470 | 1.00 | 20.87 |
| ATOM | 3592 | O   | THR | 1052 | 85.483 | 74.677 | 41.489 | 1.00 | 20.43 |
| ATOM | 3593 | N   | SER | 1053 | 86.701 | 73.608 | 39.922 | 1.00 | 23.45 |

FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 3594 | CA  | SER | 1053 | 86.453  | 72.273 | 40.460 | 1.00 | 24.39 |
| ATOM | 3595 | CB  | SER | 1053 | 85.559  | 71.492 | 39.496 | 1.00 | 25.65 |
| ATOM | 3596 | OG  | SER | 1053 | 84.344  | 72.178 | 39.258 | 1.00 | 28.54 |
| ATOM | 3597 | C   | SER | 1053 | 87.705  | 71.455 | 40.726 | 1.00 | 25.65 |
| ATOM | 3598 | O   | SER | 1053 | 88.673  | 71.514 | 39.965 | 1.00 | 26.93 |
| ATOM | 3599 | N   | ALA | 1054 | 87.663  | 70.664 | 41.796 | 1.00 | 24.99 |
| ATOM | 3600 | CA  | ALA | 1054 | 88.775  | 69.799 | 42.170 | 1.00 | 22.41 |
| ATOM | 3601 | CB  | ALA | 1054 | 88.768  | 69.564 | 43.664 | 1.00 | 21.17 |
| ATOM | 3602 | C   | ALA | 1054 | 88.636  | 68.472 | 41.438 | 1.00 | 22.07 |
| ATOM | 3603 | O   | ALA | 1054 | 87.684  | 67.729 | 41.678 | 1.00 | 24.02 |
| ATOM | 3604 | N   | LEU | 1055 | 89.562  | 68.192 | 40.527 | 1.00 | 21.30 |
| ATOM | 3605 | CA  | LEU | 1055 | 89.544  | 66.943 | 39.764 | 1.00 | 20.33 |
| ATOM | 3606 | CB  | LEU | 1055 | 90.431  | 67.057 | 38.514 | 1.00 | 17.85 |
| ATOM | 3607 | CG  | LEU | 1055 | 90.570  | 65.821 | 37.621 | 1.00 | 14.28 |
| ATOM | 3608 | CD1 | LEU | 1055 | 89.285  | 65.584 | 36.870 | 1.00 | 14.74 |
| ATOM | 3609 | CD2 | LEU | 1055 | 91.691  | 66.013 | 36.637 | 1.00 | 15.53 |
| ATOM | 3610 | C   | LEU | 1055 | 90.037  | 65.793 | 40.641 | 1.00 | 20.19 |
| ATOM | 3611 | O   | LEU | 1055 | 89.503  | 64.680 | 40.590 | 1.00 | 18.90 |
| ATOM | 3612 | N   | THR | 1056 | 91.072  | 66.069 | 41.427 | 1.00 | 20.07 |
| ATOM | 3613 | CA  | THR | 1056 | 91.663  | 65.082 | 42.316 | 1.00 | 19.85 |
| ATOM | 3614 | CB  | THR | 1056 | 92.894  | 64.409 | 41.683 | 1.00 | 18.25 |
| ATOM | 3615 | OG1 | THR | 1056 | 93.885  | 65.401 | 41.397 | 1.00 | 19.25 |
| ATOM | 3616 | CG2 | THR | 1056 | 92.531  | 63.690 | 40.403 | 1.00 | 14.77 |
| ATOM | 3617 | C   | THR | 1056 | 92.131  | 65.838 | 43.540 | 1.00 | 20.51 |
| ATOM | 3618 | O   | THR | 1056 | 91.976  | 67.058 | 43.604 | 1.00 | 21.19 |
| ATOM | 3619 | N   | LYS | 1057 | 92.722  | 65.128 | 44.497 | 1.00 | 21.94 |
| ATOM | 3620 | CA  | LYS | 1057 | 93.220  | 65.761 | 45.714 | 1.00 | 23.37 |
| ATOM | 3621 | CB  | LYS | 1057 | 93.972  | 64.764 | 46.588 | 1.00 | 21.65 |
| ATOM | 3622 | CG  | LYS | 1057 | 93.112  | 63.737 | 47.272 | 1.00 | 19.15 |
| ATOM | 3623 | CD  | LYS | 1057 | 93.705  | 63.415 | 48.622 | 1.00 | 17.97 |
| ATOM | 3624 | CE  | LYS | 1057 | 93.180  | 62.105 | 49.138 | 1.00 | 27.69 |
| ATOM | 3625 | NZ  | LYS | 1057 | 93.665  | 60.994 | 48.278 | 1.00 | 36.74 |
| ATOM | 3626 | C   | LYS | 1057 | 94.142  | 66.935 | 45.423 | 1.00 | 26.24 |
| ATOM | 3627 | O   | LYS | 1057 | 94.125  | 67.929 | 46.146 | 1.00 | 27.88 |
| ATOM | 3628 | N   | LYS | 1058 | 94.956  | 66.818 | 44.375 | 1.00 | 28.24 |
| ATOM | 3629 | CA  | LYS | 1058 | 95.876  | 67.890 | 44.021 | 1.00 | 28.47 |
| ATOM | 3630 | CB  | LYS | 1058 | 97.334  | 67.441 | 44.196 | 1.00 | 31.38 |
| ATOM | 3631 | CG  | LYS | 1058 | 97.711  | 67.172 | 45.662 | 1.00 | 35.79 |
| ATOM | 3632 | CD  | LYS | 1058 | 99.219  | 67.048 | 45.876 | 1.00 | 41.70 |
| ATOM | 3633 | CE  | LYS | 1058 | 99.818  | 65.871 | 45.107 | 1.00 | 45.88 |
| ATOM | 3634 | NZ  | LYS | 1058 | 101.284 | 65.717 | 45.357 | 1.00 | 48.09 |
| ATOM | 3635 | C   | LYS | 1058 | 95.647  | 68.564 | 42.663 | 1.00 | 27.92 |
| ATOM | 3636 | O   | LYS | 1058 | 96.298  | 69.560 | 42.352 | 1.00 | 29.57 |
| ATOM | 3637 | N   | ILE | 1059 | 94.732  | 68.040 | 41.852 | 1.00 | 26.71 |
| ATOM | 3638 | CA  | ILE | 1059 | 94.434  | 68.674 | 40.570 | 1.00 | 24.61 |
| ATOM | 3639 | CB  | ILE | 1059 | 94.403  | 67.678 | 39.404 | 1.00 | 20.79 |
| ATOM | 3640 | CG2 | ILE | 1059 | 93.915  | 68.372 | 38.142 | 1.00 | 22.24 |
| ATOM | 3641 | CG1 | ILE | 1059 | 95.800  | 67.113 | 39.159 | 1.00 | 21.03 |
| ATOM | 3642 | CD1 | ILE | 1059 | 95.930  | 66.308 | 37.874 | 1.00 | 19.39 |
| ATOM | 3643 | C   | ILE | 1059 | 93.095  | 69.415 | 40.656 | 1.00 | 25.03 |
| ATOM | 3644 | O   | ILE | 1059 | 92.101  | 68.866 | 41.137 | 1.00 | 24.20 |
| ATOM | 3645 | N   | THR | 1060 | 93.092  | 70.656 | 40.171 | 1.00 | 24.97 |
| ATOM | 3646 | CA  | THR | 1060 | 91.924  | 71.540 | 40.174 | 1.00 | 24.93 |
| ATOM | 3647 | CB  | THR | 1060 | 92.113  | 72.671 | 41.220 | 1.00 | 22.96 |
| ATOM | 3648 | OG1 | THR | 1060 | 92.137  | 72.118 | 42.541 | 1.00 | 26.30 |
| ATOM | 3649 | CG2 | THR | 1060 | 91.001  | 73.692 | 41.134 | 1.00 | 21.60 |
| ATOM | 3650 | C   | THR | 1060 | 91.789  | 72.193 | 38.795 | 1.00 | 25.85 |
| ATOM | 3651 | O   | THR | 1060 | 92.780  | 72.660 | 38.235 | 1.00 | 29.42 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3652 | N   | LEU | 1061 | 90.578 | 72.230 | 38.251 | 1.00 | 23.74 |
| ATOM | 3653 | CA  | LEU | 1061 | 90.341 | 72.831 | 36.945 | 1.00 | 21.19 |
| ATOM | 3654 | CB  | LEU | 1061 | 89.598 | 71.847 | 36.052 | 1.00 | 20.39 |
| ATOM | 3655 | CG  | LEU | 1061 | 90.136 | 70.423 | 35.971 | 1.00 | 20.17 |
| ATOM | 3656 | CD1 | LEU | 1061 | 89.053 | 69.484 | 35.447 | 1.00 | 15.54 |
| ATOM | 3657 | CD2 | LEU | 1061 | 91.367 | 70.405 | 35.085 | 1.00 | 20.41 |
| ATOM | 3658 | C   | LEU | 1061 | 89.480 | 74.067 | 37.115 | 1.00 | 22.35 |
| ATOM | 3659 | O   | LEU | 1061 | 88.876 | 74.279 | 38.171 | 1.00 | 22.51 |
| ATOM | 3660 | N   | LYS | 1062 | 89.391 | 74.867 | 36.061 | 1.00 | 24.07 |
| ATOM | 3661 | CA  | LYS | 1062 | 88.578 | 76.078 | 36.093 | 1.00 | 25.75 |
| ATOM | 3662 | CB  | LYS | 1062 | 89.028 | 77.063 | 35.008 | 1.00 | 30.52 |
| ATOM | 3663 | CG  | LYS | 1062 | 90.476 | 77.540 | 35.142 | 1.00 | 34.98 |
| ATOM | 3664 | CD  | LYS | 1062 | 90.667 | 78.567 | 36.249 | 1.00 | 35.68 |
| ATOM | 3665 | CE  | LYS | 1062 | 92.160 | 78.787 | 36.548 | 1.00 | 40.74 |
| ATOM | 3666 | NZ  | LYS | 1062 | 92.979 | 79.256 | 35.378 | 1.00 | 40.68 |
| ATOM | 3667 | C   | LYS | 1062 | 87.115 | 75.714 | 35.884 | 1.00 | 25.76 |
| ATOM | 3668 | O   | LYS | 1062 | 86.234 | 76.534 | 36.111 | 1.00 | 28.56 |
| ATOM | 3669 | N   | THR | 1063 | 86.866 | 74.503 | 35.386 | 1.00 | 26.18 |
| ATOM | 3670 | CA  | THR | 1063 | 85.509 | 74.007 | 35.154 | 1.00 | 24.51 |
| ATOM | 3671 | CB  | THR | 1063 | 85.121 | 74.068 | 33.657 | 1.00 | 22.57 |
| ATOM | 3672 | OG1 | THR | 1063 | 85.783 | 73.022 | 32.945 | 1.00 | 24.96 |
| ATOM | 3673 | CG2 | THR | 1063 | 85.509 | 75.409 | 33.054 | 1.00 | 19.73 |
| ATOM | 3674 | C   | THR | 1063 | 85.419 | 72.547 | 35.628 | 1.00 | 23.22 |
| ATOM | 3675 | O   | THR | 1063 | 86.438 | 71.909 | 35.888 | 1.00 | 24.35 |
| ATOM | 3676 | N   | PRO | 1064 | 84.204 | 72.011 | 35.781 | 1.00 | 20.91 |
| ATOM | 3677 | CD  | PRO | 1064 | 82.906 | 72.709 | 35.907 | 1.00 | 19.27 |
| ATOM | 3678 | CA  | PRO | 1064 | 84.095 | 70.623 | 36.234 | 1.00 | 18.80 |
| ATOM | 3679 | CB  | PRO | 1064 | 82.838 | 70.658 | 37.087 | 1.00 | 16.86 |
| ATOM | 3680 | CG  | PRO | 1064 | 81.969 | 71.608 | 36.332 | 1.00 | 17.27 |
| ATOM | 3681 | C   | PRO | 1064 | 83.949 | 69.618 | 35.086 | 1.00 | 18.82 |
| ATOM | 3682 | O   | PRO | 1064 | 83.593 | 68.464 | 35.310 | 1.00 | 21.11 |
| ATOM | 3683 | N   | LEU | 1065 | 84.272 | 70.034 | 33.870 | 1.00 | 17.47 |
| ATOM | 3684 | CA  | LEU | 1065 | 84.101 | 69.176 | 32.711 | 1.00 | 13.63 |
| ATOM | 3685 | CB  | LEU | 1065 | 83.717 | 70.038 | 31.507 | 1.00 | 16.00 |
| ATOM | 3686 | CG  | LEU | 1065 | 82.675 | 71.127 | 31.834 | 1.00 | 15.86 |
| ATOM | 3687 | CD1 | LEU | 1065 | 82.457 | 72.076 | 30.657 | 1.00 | 13.35 |
| ATOM | 3688 | CD2 | LEU | 1065 | 81.370 | 70.476 | 32.267 | 1.00 | 12.21 |
| ATOM | 3689 | C   | LEU | 1065 | 85.308 | 68.303 | 32.410 | 1.00 | 15.32 |
| ATOM | 3690 | O   | LEU | 1065 | 86.440 | 68.778 | 32.304 | 1.00 | 15.30 |
| ATOM | 3691 | N   | VAL | 1066 | 85.036 | 67.018 | 32.233 | 1.00 | 17.58 |
| ATOM | 3692 | CA  | VAL | 1066 | 86.052 | 66.003 | 31.962 | 1.00 | 17.87 |
| ATOM | 3693 | CB  | VAL | 1066 | 86.165 | 65.019 | 33.179 | 1.00 | 18.83 |
| ATOM | 3694 | CG1 | VAL | 1066 | 87.154 | 63.908 | 32.889 | 1.00 | 18.72 |
| ATOM | 3695 | CG2 | VAL | 1066 | 86.556 | 65.763 | 34.447 | 1.00 | 19.44 |
| ATOM | 3696 | C   | VAL | 1066 | 85.579 | 65.177 | 30.767 | 1.00 | 18.45 |
| ATOM | 3697 | O   | VAL | 1066 | 84.395 | 64.849 | 30.686 | 1.00 | 20.05 |
| ATOM | 3698 | N   | SER | 1067 | 86.470 | 64.856 | 29.834 | 1.00 | 18.12 |
| ATOM | 3699 | CA  | SER | 1067 | 86.059 | 64.027 | 28.709 | 1.00 | 19.04 |
| ATOM | 3700 | CB  | SER | 1067 | 86.741 | 64.447 | 27.401 | 1.00 | 17.98 |
| ATOM | 3701 | OG  | SER | 1067 | 88.120 | 64.138 | 27.393 | 1.00 | 24.06 |
| ATOM | 3702 | C   | SER | 1067 | 86.343 | 62.564 | 29.060 | 1.00 | 19.98 |
| ATOM | 3703 | O   | SER | 1067 | 87.329 | 62.249 | 29.739 | 1.00 | 19.91 |
| ATOM | 3704 | N   | SER | 1068 | 85.432 | 61.688 | 28.651 | 1.00 | 20.10 |
| ATOM | 3705 | CA  | SER | 1068 | 85.535 | 60.264 | 28.925 | 1.00 | 20.27 |
| ATOM | 3706 | CB  | SER | 1068 | 84.174 | 59.597 | 28.708 | 1.00 | 24.52 |
| ATOM | 3707 | OG  | SER | 1068 | 84.224 | 58.192 | 28.931 | 1.00 | 26.68 |
| ATOM | 3708 | C   | SER | 1068 | 86.569 | 59.557 | 28.081 | 1.00 | 20.17 |
| ATOM | 3709 | O   | SER | 1068 | 86.617 | 59.743 | 26.865 | 1.00 | 21.59 |



FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3710 | N   | PRO | 1069 | 87.392 | 58.706 | 28.710 | 1.00 | 19.67 |
| ATOM | 3711 | CD  | PRO | 1069 | 87.490 | 58.496 | 30.167 | 1.00 | 18.49 |
| ATOM | 3712 | CA  | PRO | 1069 | 88.430 | 57.953 | 28.009 | 1.00 | 18.30 |
| ATOM | 3713 | CB  | PRO | 1069 | 89.249 | 57.373 | 29.158 | 1.00 | 17.03 |
| ATOM | 3714 | CG  | PRO | 1069 | 88.245 | 57.203 | 30.248 | 1.00 | 15.39 |
| ATOM | 3715 | C   | PRO | 1069 | 87.805 | 56.852 | 27.153 | 1.00 | 20.15 |
| ATOM | 3716 | O   | PRO | 1069 | 87.676 | 55.707 | 27.588 | 1.00 | 22.07 |
| ATOM | 3717 | N   | MET | 1070 | 87.384 | 57.209 | 25.948 | 1.00 | 20.29 |
| ATOM | 3718 | CA  | MET | 1070 | 86.770 | 56.254 | 25.035 | 1.00 | 20.57 |
| ATOM | 3719 | CB  | MET | 1070 | 85.254 | 56.423 | 25.053 | 1.00 | 20.27 |
| ATOM | 3720 | CG  | MET | 1070 | 84.621 | 56.059 | 26.379 | 1.00 | 21.67 |
| ATOM | 3721 | SD  | MET | 1070 | 82.879 | 56.473 | 26.451 | 1.00 | 21.01 |
| ATOM | 3722 | CE  | MET | 1070 | 82.210 | 55.085 | 25.547 | 1.00 | 20.49 |
| ATOM | 3723 | C   | MET | 1070 | 87.331 | 56.501 | 23.641 | 1.00 | 22.45 |
| ATOM | 3724 | O   | MET | 1070 | 87.575 | 57.650 | 23.261 | 1.00 | 20.92 |
| ATOM | 3725 | N   | ASP | 1071 | 87.515 | 55.432 | 22.867 | 1.00 | 24.82 |
| ATOM | 3726 | CA  | ASP | 1071 | 88.092 | 55.573 | 21.533 | 1.00 | 25.66 |
| ATOM | 3727 | CB  | ASP | 1071 | 88.454 | 54.216 | 20.894 | 1.00 | 27.27 |
| ATOM | 3728 | CG  | ASP | 1071 | 87.308 | 53.226 | 20.881 | 1.00 | 31.83 |
| ATOM | 3729 | OD1 | ASP | 1071 | 86.158 | 53.615 | 20.588 | 1.00 | 37.06 |
| ATOM | 3730 | OD2 | ASP | 1071 | 87.574 | 52.035 | 21.143 | 1.00 | 33.11 |
| ATOM | 3731 | C   | ASP | 1071 | 87.367 | 56.478 | 20.549 | 1.00 | 24.21 |
| ATOM | 3732 | O   | ASP | 1071 | 87.972 | 56.939 | 19.587 | 1.00 | 25.35 |
| ATOM | 3733 | N   | THR | 1072 | 86.092 | 56.752 | 20.797 | 1.00 | 24.00 |
| ATOM | 3734 | CA  | THR | 1072 | 85.327 | 57.638 | 19.924 | 1.00 | 22.90 |
| ATOM | 3735 | CB  | THR | 1072 | 84.036 | 56.961 | 19.415 | 1.00 | 19.61 |
| ATOM | 3736 | OG1 | THR | 1072 | 83.200 | 56.592 | 20.524 | 1.00 | 16.40 |
| ATOM | 3737 | CG2 | THR | 1072 | 84.378 | 55.728 | 18.621 | 1.00 | 18.17 |
| ATOM | 3738 | C   | THR | 1072 | 84.980 | 58.947 | 20.641 | 1.00 | 23.02 |
| ATOM | 3739 | O   | THR | 1072 | 84.010 | 59.624 | 20.289 | 1.00 | 24.03 |
| ATOM | 3740 | N   | VAL | 1073 | 85.766 | 59.292 | 21.658 | 1.00 | 22.41 |
| ATOM | 3741 | CA  | VAL | 1073 | 85.529 | 60.510 | 22.420 | 1.00 | 21.20 |
| ATOM | 3742 | CB  | VAL | 1073 | 84.752 | 60.229 | 23.741 | 1.00 | 19.24 |
| ATOM | 3743 | CG1 | VAL | 1073 | 84.571 | 61.504 | 24.535 | 1.00 | 17.63 |
| ATOM | 3744 | CG2 | VAL | 1073 | 83.394 | 59.641 | 23.452 | 1.00 | 16.74 |
| ATOM | 3745 | C   | VAL | 1073 | 86.823 | 61.232 | 22.764 | 1.00 | 22.61 |
| ATOM | 3746 | O   | VAL | 1073 | 86.969 | 62.417 | 22.477 | 1.00 | 22.14 |
| ATOM | 3747 | N   | THR | 1074 | 87.793 | 60.516 | 23.318 | 1.00 | 24.79 |
| ATOM | 3748 | CA  | THR | 1074 | 89.025 | 61.187 | 23.708 | 1.00 | 26.86 |
| ATOM | 3749 | CB  | THR | 1074 | 89.104 | 61.359 | 25.247 | 1.00 | 29.38 |
| ATOM | 3750 | OG1 | THR | 1074 | 87.865 | 61.893 | 25.735 | 1.00 | 32.73 |
| ATOM | 3751 | CG2 | THR | 1074 | 90.217 | 62.324 | 25.622 | 1.00 | 30.82 |
| ATOM | 3752 | C   | THR | 1074 | 90.370 | 60.686 | 23.199 | 1.00 | 26.15 |
| ATOM | 3753 | O   | THR | 1074 | 90.750 | 59.529 | 23.380 | 1.00 | 25.91 |
| ATOM | 3754 | N   | GLU | 1075 | 91.091 | 61.622 | 22.595 | 1.00 | 28.59 |
| ATOM | 3755 | CA  | GLU | 1075 | 92.431 | 61.443 | 22.059 | 1.00 | 31.08 |
| ATOM | 3756 | CB  | GLU | 1075 | 92.402 | 60.912 | 20.627 | 1.00 | 30.41 |
| ATOM | 3757 | CG  | GLU | 1075 | 92.244 | 59.400 | 20.558 | 1.00 | 29.53 |
| ATOM | 3758 | CD  | GLU | 1075 | 92.481 | 58.825 | 19.178 | 1.00 | 30.14 |
| ATOM | 3759 | OE1 | GLU | 1075 | 92.098 | 57.659 | 18.958 | 1.00 | 32.49 |
| ATOM | 3760 | OE2 | GLU | 1075 | 93.059 | 59.519 | 18.314 | 1.00 | 33.89 |
| ATOM | 3761 | C   | GLU | 1075 | 93.065 | 62.833 | 22.121 | 1.00 | 34.13 |
| ATOM | 3762 | O   | GLU | 1075 | 92.462 | 63.751 | 22.683 | 1.00 | 36.70 |
| ATOM | 3763 | N   | ALA | 1076 | 94.251 | 63.002 | 21.538 | 1.00 | 35.59 |
| ATOM | 3764 | CA  | ALA | 1076 | 94.956 | 64.292 | 21.570 | 1.00 | 35.10 |
| ATOM | 3765 | CB  | ALA | 1076 | 96.151 | 64.275 | 20.620 | 1.00 | 35.89 |
| ATOM | 3766 | C   | ALA | 1076 | 94.100 | 65.532 | 21.319 | 1.00 | 34.42 |
| ATOM | 3767 | O   | ALA | 1076 | 93.986 | 66.389 | 22.194 | 1.00 | 34.97 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3768 | N   | GLY | 1077 | 93.480 | 65.613 | 20.144 | 1.00 | 34.10 |
| ATOM | 3769 | CA  | GLY | 1077 | 92.655 | 66.763 | 19.810 | 1.00 | 34.49 |
| ATOM | 3770 | C   | GLY | 1077 | 91.655 | 67.146 | 20.886 | 1.00 | 35.44 |
| ATOM | 3771 | O   | GLY | 1077 | 91.574 | 68.314 | 21.278 | 1.00 | 35.30 |
| ATOM | 3772 | N   | MET | 1078 | 90.895 | 66.159 | 21.356 | 1.00 | 35.00 |
| ATOM | 3773 | CA  | MET | 1078 | 89.892 | 66.361 | 22.400 | 1.00 | 32.60 |
| ATOM | 3774 | CB  | MET | 1078 | 89.122 | 65.060 | 22.650 | 1.00 | 30.21 |
| ATOM | 3775 | CG  | MET | 1078 | 88.115 | 65.119 | 23.787 | 1.00 | 23.97 |
| ATOM | 3776 | SD  | MET | 1078 | 86.729 | 66.180 | 23.420 | 1.00 | 22.65 |
| ATOM | 3777 | CE  | MET | 1078 | 85.882 | 65.186 | 22.153 | 1.00 | 13.83 |
| ATOM | 3778 | C   | MET | 1078 | 90.562 | 66.806 | 23.691 | 1.00 | 32.54 |
| ATOM | 3779 | O   | MET | 1078 | 90.281 | 67.890 | 24.205 | 1.00 | 33.25 |
| ATOM | 3780 | N   | ALA | 1079 | 91.473 | 65.975 | 24.191 | 1.00 | 29.80 |
| ATOM | 3781 | CA  | ALA | 1079 | 92.185 | 66.264 | 25.426 | 1.00 | 26.90 |
| ATOM | 3782 | CB  | ALA | 1079 | 93.312 | 65.272 | 25.625 | 1.00 | 25.36 |
| ATOM | 3783 | C   | ALA | 1079 | 92.719 | 67.686 | 25.411 | 1.00 | 26.03 |
| ATOM | 3784 | O   | ALA | 1079 | 92.675 | 68.385 | 26.426 | 1.00 | 25.26 |
| ATOM | 3785 | N   | ILE | 1080 | 93.163 | 68.132 | 24.238 | 1.00 | 26.03 |
| ATOM | 3786 | CA  | ILE | 1080 | 93.696 | 69.481 | 24.082 | 1.00 | 25.73 |
| ATOM | 3787 | CB  | ILE | 1080 | 94.486 | 69.632 | 22.761 | 1.00 | 23.56 |
| ATOM | 3788 | CG2 | ILE | 1080 | 94.898 | 71.086 | 22.540 | 1.00 | 22.24 |
| ATOM | 3789 | CG1 | ILE | 1080 | 95.740 | 68.763 | 22.810 | 1.00 | 21.45 |
| ATOM | 3790 | CD1 | ILE | 1080 | 96.565 | 68.809 | 21.554 | 1.00 | 22.68 |
| ATOM | 3791 | C   | ILE | 1080 | 92.587 | 70.530 | 24.154 | 1.00 | 26.48 |
| ATOM | 3792 | O   | ILE | 1080 | 92.645 | 71.444 | 24.979 | 1.00 | 25.96 |
| ATOM | 3793 | N   | ALA | 1081 | 91.559 | 70.369 | 23.323 | 1.00 | 27.21 |
| ATOM | 3794 | CA  | ALA | 1081 | 90.438 | 71.305 | 23.285 | 1.00 | 25.13 |
| ATOM | 3795 | CB  | ALA | 1081 | 89.422 | 70.866 | 22.240 | 1.00 | 23.36 |
| ATOM | 3796 | C   | ALA | 1081 | 89.778 | 71.410 | 24.652 | 1.00 | 25.14 |
| ATOM | 3797 | O   | ALA | 1081 | 89.335 | 72.484 | 25.064 | 1.00 | 26.40 |
| ATOM | 3798 | N   | MET | 1082 | 89.762 | 70.295 | 25.369 | 1.00 | 25.59 |
| ATOM | 3799 | CA  | MET | 1082 | 89.162 | 70.232 | 26.691 | 1.00 | 26.26 |
| ATOM | 3800 | CB  | MET | 1082 | 89.051 | 68.771 | 27.146 | 1.00 | 27.01 |
| ATOM | 3801 | CG  | MET | 1082 | 87.856 | 68.464 | 28.048 | 1.00 | 28.65 |
| ATOM | 3802 | SD  | MET | 1082 | 86.249 | 68.526 | 27.203 | 1.00 | 26.79 |
| ATOM | 3803 | CE  | MET | 1082 | 85.315 | 69.478 | 28.353 | 1.00 | 23.90 |
| ATOM | 3804 | C   | MET | 1082 | 89.992 | 71.056 | 27.675 | 1.00 | 25.81 |
| ATOM | 3805 | O   | MET | 1082 | 89.442 | 71.851 | 28.434 | 1.00 | 26.89 |
| ATOM | 3806 | N   | ALA | 1083 | 91.314 | 70.913 | 27.624 | 1.00 | 25.36 |
| ATOM | 3807 | CA  | ALA | 1083 | 92.195 | 71.663 | 28.519 | 1.00 | 23.07 |
| ATOM | 3808 | CB  | ALA | 1083 | 93.594 | 71.105 | 28.472 | 1.00 | 19.47 |
| ATOM | 3809 | C   | ALA | 1083 | 92.217 | 73.158 | 28.205 | 1.00 | 24.00 |
| ATOM | 3810 | O   | ALA | 1083 | 92.330 | 73.990 | 29.107 | 1.00 | 23.89 |
| ATOM | 3811 | N   | LEU | 1084 | 92.117 | 73.508 | 26.927 | 1.00 | 24.04 |
| ATOM | 3812 | CA  | LEU | 1084 | 92.133 | 74.913 | 26.550 | 1.00 | 21.88 |
| ATOM | 3813 | CB  | LEU | 1084 | 92.278 | 75.092 | 25.031 | 1.00 | 20.51 |
| ATOM | 3814 | CG  | LEU | 1084 | 93.621 | 74.803 | 24.333 | 1.00 | 17.98 |
| ATOM | 3815 | CD1 | LEU | 1084 | 93.489 | 75.021 | 22.834 | 1.00 | 10.91 |
| ATOM | 3816 | CD2 | LEU | 1084 | 94.728 | 75.687 | 24.892 | 1.00 | 16.24 |
| ATOM | 3817 | C   | LEU | 1084 | 90.872 | 75.603 | 27.038 | 1.00 | 23.28 |
| ATOM | 3818 | O   | LEU | 1084 | 90.939 | 76.749 | 27.472 | 1.00 | 24.38 |
| ATOM | 3819 | N   | THR | 1085 | 89.738 | 74.897 | 27.009 | 1.00 | 23.36 |
| ATOM | 3820 | CA  | THR | 1085 | 88.458 | 75.477 | 27.433 | 1.00 | 22.95 |
| ATOM | 3821 | CB  | THR | 1085 | 87.267 | 74.937 | 26.604 | 1.00 | 20.99 |
| ATOM | 3822 | OG1 | THR | 1085 | 87.256 | 73.508 | 26.631 | 1.00 | 25.05 |
| ATOM | 3823 | CG2 | THR | 1085 | 87.370 | 75.410 | 25.176 | 1.00 | 16.76 |
| ATOM | 3824 | C   | THR | 1085 | 88.117 | 75.425 | 28.921 | 1.00 | 23.92 |
| ATOM | 3825 | O   | THR | 1085 | 87.077 | 75.954 | 29.342 | 1.00 | 25.16 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3826 | N   | GLY | 1086 | 88.973 | 74.791 | 29.716 | 1.00 | 24.85 |
| ATOM | 3827 | CA  | GLY | 1086 | 88.731 | 74.748 | 31.150 | 1.00 | 26.30 |
| ATOM | 3828 | C   | GLY | 1086 | 88.614 | 73.400 | 31.835 | 1.00 | 25.84 |
| ATOM | 3829 | O   | GLY | 1086 | 88.517 | 73.336 | 33.063 | 1.00 | 26.47 |
| ATOM | 3830 | N   | GLY | 1087 | 88.570 | 72.332 | 31.057 | 1.00 | 25.34 |
| ATOM | 3831 | CA  | GLY | 1087 | 88.464 | 71.013 | 31.641 | 1.00 | 24.99 |
| ATOM | 3832 | C   | GLY | 1087 | 89.723 | 70.212 | 31.406 | 1.00 | 24.03 |
| ATOM | 3833 | O   | GLY | 1087 | 90.823 | 70.761 | 31.358 | 1.00 | 23.72 |
| ATOM | 3834 | N   | ILE | 1088 | 89.555 | 68.908 | 31.244 | 1.00 | 23.71 |
| ATOM | 3835 | CA  | ILE | 1088 | 90.673 | 68.007 | 31.006 | 1.00 | 23.17 |
| ATOM | 3836 | CB  | ILE | 1088 | 91.360 | 67.582 | 32.352 | 1.00 | 20.71 |
| ATOM | 3837 | CG2 | ILE | 1088 | 90.444 | 66.669 | 33.153 | 1.00 | 20.78 |
| ATOM | 3838 | CG1 | ILE | 1088 | 92.706 | 66.886 | 32.090 | 1.00 | 17.22 |
| ATOM | 3839 | CD1 | ILE | 1088 | 93.545 | 66.593 | 33.353 | 1.00 | 5.96  |
| ATOM | 3840 | C   | ILE | 1088 | 90.083 | 66.799 | 30.283 | 1.00 | 22.59 |
| ATOM | 3841 | O   | ILE | 1088 | 88.862 | 66.605 | 30.281 | 1.00 | 22.13 |
| ATOM | 3842 | N   | GLY | 1089 | 90.939 | 66.023 | 29.630 | 1.00 | 22.64 |
| ATOM | 3843 | CA  | GLY | 1089 | 90.476 | 64.853 | 28.912 | 1.00 | 21.60 |
| ATOM | 3844 | C   | GLY | 1089 | 91.292 | 63.622 | 29.250 | 1.00 | 22.41 |
| ATOM | 3845 | O   | GLY | 1089 | 92.433 | 63.728 | 29.697 | 1.00 | 22.07 |
| ATOM | 3846 | N   | PHE | 1090 | 90.702 | 62.449 | 29.068 | 1.00 | 22.64 |
| ATOM | 3847 | CA  | PHE | 1090 | 91.403 | 61.215 | 29.350 | 1.00 | 22.39 |
| ATOM | 3848 | CB  | PHE | 1090 | 90.668 | 60.425 | 30.423 | 1.00 | 24.55 |
| ATOM | 3849 | CG  | PHE | 1090 | 90.775 | 61.026 | 31.782 | 1.00 | 27.69 |
| ATOM | 3850 | CD1 | PHE | 1090 | 89.903 | 62.032 | 32.181 | 1.00 | 28.68 |
| ATOM | 3851 | CD2 | PHE | 1090 | 91.775 | 60.616 | 32.658 | 1.00 | 26.87 |
| ATOM | 3852 | CE1 | PHE | 1090 | 90.034 | 62.628 | 33.439 | 1.00 | 29.16 |
| ATOM | 3853 | CE2 | PHE | 1090 | 91.912 | 61.207 | 33.917 | 1.00 | 26.20 |
| ATOM | 3854 | CZ  | PHE | 1090 | 91.041 | 62.214 | 34.304 | 1.00 | 29.03 |
| ATOM | 3855 | C   | PHE | 1090 | 91.568 | 60.380 | 28.096 | 1.00 | 22.82 |
| ATOM | 3856 | O   | PHE | 1090 | 90.579 | 59.940 | 27.511 | 1.00 | 23.69 |
| ATOM | 3857 | N   | ILE | 1091 | 92.816 | 60.191 | 27.668 | 1.00 | 21.96 |
| ATOM | 3858 | CA  | ILE | 1091 | 93.114 | 59.394 | 26.480 | 1.00 | 20.77 |
| ATOM | 3859 | CB  | ILE | 1091 | 94.633 | 59.423 | 26.128 | 1.00 | 19.10 |
| ATOM | 3860 | CG2 | ILE | 1091 | 94.892 | 58.635 | 24.846 | 1.00 | 15.49 |
| ATOM | 3861 | CG1 | ILE | 1091 | 95.147 | 60.867 | 25.999 | 1.00 | 13.00 |
| ATOM | 3862 | CD1 | ILE | 1091 | 94.662 | 61.607 | 24.779 | 1.00 | 9.34  |
| ATOM | 3863 | C   | ILE | 1091 | 92.722 | 57.950 | 26.795 | 1.00 | 20.88 |
| ATOM | 3864 | O   | ILE | 1091 | 92.958 | 57.464 | 27.907 | 1.00 | 21.15 |
| ATOM | 3865 | N   | HIS | 1092 | 92.101 | 57.276 | 25.832 | 1.00 | 21.96 |
| ATOM | 3866 | CA  | HIS | 1092 | 91.686 | 55.882 | 26.019 | 1.00 | 23.97 |
| ATOM | 3867 | CB  | HIS | 1092 | 90.613 | 55.492 | 24.994 | 1.00 | 23.05 |
| ATOM | 3868 | CG  | HIS | 1092 | 91.114 | 55.427 | 23.584 | 1.00 | 18.52 |
| ATOM | 3869 | CD2 | HIS | 1092 | 91.563 | 54.381 | 22.849 | 1.00 | 13.17 |
| ATOM | 3870 | ND1 | HIS | 1092 | 91.196 | 56.534 | 22.768 | 1.00 | 15.63 |
| ATOM | 3871 | CE1 | HIS | 1092 | 91.672 | 56.173 | 21.592 | 1.00 | 14.27 |
| ATOM | 3872 | NE2 | HIS | 1092 | 91.908 | 54.873 | 21.614 | 1.00 | 12.20 |
| ATOM | 3873 | C   | HIS | 1092 | 92.887 | 54.946 | 25.895 | 1.00 | 25.60 |
| ATOM | 3874 | O   | HIS | 1092 | 93.957 | 55.369 | 25.467 | 1.00 | 28.13 |
| ATOM | 3875 | N   | HIS | 1093 | 92.708 | 53.675 | 26.242 | 1.00 | 26.03 |
| ATOM | 3876 | CA  | HIS | 1093 | 93.805 | 52.715 | 26.139 | 1.00 | 27.95 |
| ATOM | 3877 | CB  | HIS | 1093 | 94.247 | 52.205 | 27.515 | 1.00 | 29.78 |
| ATOM | 3878 | CG  | HIS | 1093 | 93.231 | 51.358 | 28.218 | 1.00 | 33.05 |
| ATOM | 3879 | CD2 | HIS | 1093 | 93.243 | 50.043 | 28.548 | 1.00 | 34.27 |
| ATOM | 3880 | ND1 | HIS | 1093 | 92.056 | 51.867 | 28.728 | 1.00 | 33.28 |
| ATOM | 3881 | CE1 | HIS | 1093 | 91.388 | 50.906 | 29.338 | 1.00 | 32.87 |
| ATOM | 3882 | NE2 | HIS | 1093 | 92.088 | 49.790 | 29.245 | 1.00 | 34.75 |
| ATOM | 3883 | C   | HIS | 1093 | 93.518 | 51.557 | 25.193 | 1.00 | 28.37 |

FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 3884 | O   | HIS | 1093 | 94.052  | 50.467 | 25.351 | 1.00 | 26.48 |
| ATOM | 3885 | N   | ASN | 1094 | 92.596  | 51.785 | 24.265 | 1.00 | 30.84 |
| ATOM | 3886 | CA  | ASN | 1094 | 92.241  | 50.807 | 23.237 | 1.00 | 32.45 |
| ATOM | 3887 | CB  | ASN | 1094 | 90.769  | 50.963 | 22.842 | 1.00 | 35.56 |
| ATOM | 3888 | CG  | ASN | 1094 | 90.371  | 50.081 | 21.671 | 1.00 | 39.33 |
| ATOM | 3889 | OD1 | ASN | 1094 | 89.850  | 50.568 | 20.668 | 1.00 | 43.29 |
| ATOM | 3890 | ND2 | ASN | 1094 | 90.594  | 48.780 | 21.800 | 1.00 | 38.01 |
| ATOM | 3891 | C   | ASN | 1094 | 93.158  | 51.228 | 22.090 | 1.00 | 33.74 |
| ATOM | 3892 | O   | ASN | 1094 | 92.722  | 51.794 | 21.079 | 1.00 | 34.48 |
| ATOM | 3893 | N   | CYS | 1095 | 94.451  | 51.061 | 22.345 | 1.00 | 33.96 |
| ATOM | 3894 | CA  | CYS | 1095 | 95.517  | 51.431 | 21.427 | 1.00 | 32.91 |
| ATOM | 3895 | CB  | CYS | 1095 | 95.534  | 52.950 | 21.271 | 1.00 | 31.80 |
| ATOM | 3896 | SG  | CYS | 1095 | 95.537  | 53.866 | 22.840 | 1.00 | 33.34 |
| ATOM | 3897 | C   | CYS | 1095 | 96.829  | 50.961 | 22.057 | 1.00 | 33.35 |
| ATOM | 3898 | O   | CYS | 1095 | 96.876  | 50.692 | 23.257 | 1.00 | 34.13 |
| ATOM | 3899 | N   | THR | 1096 | 97.889  | 50.860 | 21.257 | 1.00 | 32.75 |
| ATOM | 3900 | CA  | THR | 1096 | 99.185  | 50.411 | 21.762 | 1.00 | 30.51 |
| ATOM | 3901 | CB  | THR | 1096 | 100.229 | 50.384 | 20.647 | 1.00 | 31.43 |
| ATOM | 3902 | OG1 | THR | 1096 | 100.530 | 51.722 | 20.243 | 1.00 | 34.77 |
| ATOM | 3903 | CG2 | THR | 1096 | 99.706  | 49.629 | 19.445 | 1.00 | 34.07 |
| ATOM | 3904 | C   | THR | 1096 | 99.659  | 51.379 | 22.835 | 1.00 | 28.94 |
| ATOM | 3905 | O   | THR | 1096 | 99.314  | 52.558 | 22.793 | 1.00 | 30.80 |
| ATOM | 3906 | N   | PRO | 1097 | 100.461 | 50.902 | 23.807 | 1.00 | 28.40 |
| ATOM | 3907 | CD  | PRO | 1097 | 100.925 | 49.519 | 24.021 | 1.00 | 28.11 |
| ATOM | 3908 | CA  | PRO | 1097 | 100.958 | 51.781 | 24.869 | 1.00 | 27.84 |
| ATOM | 3909 | CB  | PRO | 1097 | 101.916 | 50.878 | 25.632 | 1.00 | 26.37 |
| ATOM | 3910 | CG  | PRO | 1097 | 101.293 | 49.531 | 25.481 | 1.00 | 25.06 |
| ATOM | 3911 | C   | PRO | 1097 | 101.689 | 52.956 | 24.258 | 1.00 | 29.88 |
| ATOM | 3912 | O   | PRO | 1097 | 101.583 | 54.084 | 24.739 | 1.00 | 30.91 |
| ATOM | 3913 | N   | GLU | 1098 | 102.384 | 52.683 | 23.156 | 1.00 | 32.60 |
| ATOM | 3914 | CA  | GLU | 1098 | 103.153 | 53.686 | 22.420 | 1.00 | 35.02 |
| ATOM | 3915 | CB  | GLU | 1098 | 103.974 | 53.017 | 21.310 | 1.00 | 37.79 |
| ATOM | 3916 | CG  | GLU | 1098 | 105.119 | 52.122 | 21.796 | 1.00 | 44.17 |
| ATOM | 3917 | CD  | GLU | 1098 | 104.669 | 50.740 | 22.271 | 1.00 | 48.86 |
| ATOM | 3918 | OE1 | GLU | 1098 | 103.779 | 50.132 | 21.628 | 1.00 | 49.58 |
| ATOM | 3919 | OE2 | GLU | 1098 | 105.229 | 50.256 | 23.281 | 1.00 | 49.09 |
| ATOM | 3920 | C   | GLU | 1098 | 102.269 | 54.787 | 21.814 | 1.00 | 35.22 |
| ATOM | 3921 | O   | GLU | 1098 | 102.590 | 55.975 | 21.907 | 1.00 | 35.11 |
| ATOM | 3922 | N   | PHE | 1099 | 101.170 | 54.378 | 21.182 | 1.00 | 34.71 |
| ATOM | 3923 | CA  | PHE | 1099 | 100.217 | 55.295 | 20.550 | 1.00 | 31.99 |
| ATOM | 3924 | CB  | PHE | 1099 | 99.114  | 54.487 | 19.854 | 1.00 | 30.86 |
| ATOM | 3925 | CG  | PHE | 1099 | 97.961  | 55.316 | 19.356 | 1.00 | 30.84 |
| ATOM | 3926 | CD1 | PHE | 1099 | 97.896  | 55.708 | 18.027 | 1.00 | 30.84 |
| ATOM | 3927 | CD2 | PHE | 1099 | 96.906  | 55.654 | 20.203 | 1.00 | 30.22 |
| ATOM | 3928 | CE1 | PHE | 1099 | 96.795  | 56.418 | 17.543 | 1.00 | 32.30 |
| ATOM | 3929 | CE2 | PHE | 1099 | 95.807  | 56.360 | 19.730 | 1.00 | 29.93 |
| ATOM | 3930 | CZ  | PHE | 1099 | 95.750  | 56.742 | 18.395 | 1.00 | 30.84 |
| ATOM | 3931 | C   | PHE | 1099 | 99.591  | 56.202 | 21.591 | 1.00 | 30.63 |
| ATOM | 3932 | O   | PHE | 1099 | 99.468  | 57.412 | 21.385 | 1.00 | 29.46 |
| ATOM | 3933 | N   | GLN | 1100 | 99.169  | 55.592 | 22.694 | 1.00 | 31.39 |
| ATOM | 3934 | CA  | GLN | 1100 | 98.535  | 56.312 | 23.782 | 1.00 | 33.54 |
| ATOM | 3935 | CB  | GLN | 1100 | 98.087  | 55.341 | 24.873 | 1.00 | 33.46 |
| ATOM | 3936 | CG  | GLN | 1100 | 97.206  | 56.000 | 25.918 | 1.00 | 33.43 |
| ATOM | 3937 | CD  | GLN | 1100 | 96.860  | 55.082 | 27.061 | 1.00 | 31.11 |
| ATOM | 3938 | OE1 | GLN | 1100 | 97.552  | 54.111 | 27.321 | 1.00 | 30.24 |
| ATOM | 3939 | NE2 | GLN | 1100 | 95.784  | 55.397 | 27.765 | 1.00 | 34.07 |
| ATOM | 3940 | C   | GLN | 1100 | 99.497  | 57.342 | 24.354 | 1.00 | 35.00 |
| ATOM | 3941 | O   | GLN | 1100 | 99.145  | 58.518 | 24.499 | 1.00 | 35.07 |

FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 3942 | N   | ALA | 1101 | 100.714 | 56.895 | 24.665 | 1.00 | 35.47 |
| ATOM | 3943 | CA  | ALA | 1101 | 101.752 | 57.772 | 25.206 | 1.00 | 34.10 |
| ATOM | 3944 | CB  | ALA | 1101 | 103.010 | 56.973 | 25.524 | 1.00 | 34.60 |
| ATOM | 3945 | C   | ALA | 1101 | 102.062 | 58.868 | 24.192 | 1.00 | 33.13 |
| ATOM | 3946 | O   | ALA | 1101 | 102.335 | 60.008 | 24.564 | 1.00 | 33.43 |
| ATOM | 3947 | N   | ASN | 1102 | 102.004 | 58.515 | 22.911 | 1.00 | 31.74 |
| ATOM | 3948 | CA  | ASN | 1102 | 102.251 | 59.464 | 21.831 | 1.00 | 31.93 |
| ATOM | 3949 | CB  | ASN | 1102 | 102.220 | 58.754 | 20.478 | 1.00 | 35.75 |
| ATOM | 3950 | CG  | ASN | 1102 | 102.222 | 59.722 | 19.314 | 1.00 | 38.97 |
| ATOM | 3951 | OD1 | ASN | 1102 | 103.115 | 60.562 | 19.188 | 1.00 | 35.68 |
| ATOM | 3952 | ND2 | ASN | 1102 | 101.207 | 59.617 | 18.460 | 1.00 | 44.14 |
| ATOM | 3953 | C   | ASN | 1102 | 101.174 | 60.535 | 21.878 | 1.00 | 30.58 |
| ATOM | 3954 | O   | ASN | 1102 | 101.465 | 61.734 | 21.820 | 1.00 | 28.72 |
| ATOM | 3955 | N   | GLU | 1103 | 99.926  | 60.092 | 21.994 | 1.00 | 30.88 |
| ATOM | 3956 | CA  | GLU | 1103 | 98.797  | 61.008 | 22.081 | 1.00 | 31.29 |
| ATOM | 3957 | CB  | GLU | 1103 | 97.496  | 60.236 | 22.305 | 1.00 | 29.94 |
| ATOM | 3958 | CG  | GLU | 1103 | 97.107  | 59.345 | 21.143 | 1.00 | 26.07 |
| ATOM | 3959 | CD  | GLU | 1103 | 97.147  | 60.077 | 19.817 | 1.00 | 26.39 |
| ATOM | 3960 | OE1 | GLU | 1103 | 96.367  | 61.041 | 19.642 | 1.00 | 23.03 |
| ATOM | 3961 | OE2 | GLU | 1103 | 97.972  | 59.695 | 18.957 | 1.00 | 27.36 |
| ATOM | 3962 | C   | GLU | 1103 | 99.033  | 61.971 | 23.236 | 1.00 | 31.53 |
| ATOM | 3963 | O   | GLU | 1103 | 98.880  | 63.183 | 23.077 | 1.00 | 32.08 |
| ATOM | 3964 | N   | VAL | 1104 | 99.448  | 61.421 | 24.378 | 1.00 | 32.16 |
| ATOM | 3965 | CA  | VAL | 1104 | 99.731  | 62.201 | 25.585 | 1.00 | 33.27 |
| ATOM | 3966 | CB  | VAL | 1104 | 100.191 | 61.286 | 26.744 | 1.00 | 30.58 |
| ATOM | 3967 | CG1 | VAL | 1104 | 100.569 | 62.110 | 27.962 | 1.00 | 28.79 |
| ATOM | 3968 | CG2 | VAL | 1104 | 99.093  | 60.304 | 27.096 | 1.00 | 32.06 |
| ATOM | 3969 | C   | VAL | 1104 | 100.823 | 63.225 | 25.306 | 1.00 | 34.57 |
| ATOM | 3970 | O   | VAL | 1104 | 100.695 | 64.404 | 25.649 | 1.00 | 34.06 |
| ATOM | 3971 | N   | ARG | 1105 | 101.876 | 62.762 | 24.642 | 1.00 | 36.12 |
| ATOM | 3972 | CA  | ARG | 1105 | 103.020 | 63.591 | 24.291 | 1.00 | 37.17 |
| ATOM | 3973 | CB  | ARG | 1105 | 103.981 | 62.780 | 23.422 | 1.00 | 41.18 |
| ATOM | 3974 | CG  | ARG | 1105 | 105.100 | 63.589 | 22.822 | 1.00 | 48.61 |
| ATOM | 3975 | CD  | ARG | 1105 | 105.767 | 62.842 | 21.689 | 1.00 | 54.64 |
| ATOM | 3976 | NE  | ARG | 1105 | 106.570 | 63.746 | 20.872 | 1.00 | 59.97 |
| ATOM | 3977 | CZ  | ARG | 1105 | 106.096 | 64.448 | 19.845 | 1.00 | 63.88 |
| ATOM | 3978 | NH1 | ARG | 1105 | 104.816 | 64.349 | 19.494 | 1.00 | 63.25 |
| ATOM | 3979 | NH2 | ARG | 1105 | 106.899 | 65.269 | 19.180 | 1.00 | 67.43 |
| ATOM | 3980 | C   | ARG | 1105 | 102.572 | 64.848 | 23.552 | 1.00 | 35.76 |
| ATOM | 3981 | O   | ARG | 1105 | 102.880 | 65.968 | 23.966 | 1.00 | 34.77 |
| ATOM | 3982 | N   | LYS | 1106 | 101.805 | 64.649 | 22.485 | 1.00 | 34.78 |
| ATOM | 3983 | CA  | LYS | 1106 | 101.301 | 65.747 | 21.669 | 1.00 | 34.00 |
| ATOM | 3984 | CB  | LYS | 1106 | 100.467 | 65.198 | 20.514 | 1.00 | 32.67 |
| ATOM | 3985 | CG  | LYS | 1106 | 101.212 | 64.189 | 19.670 | 1.00 | 31.83 |
| ATOM | 3986 | CD  | LYS | 1106 | 100.416 | 63.780 | 18.457 | 1.00 | 34.20 |
| ATOM | 3987 | CE  | LYS | 1106 | 99.090  | 63.176 | 18.846 | 1.00 | 39.46 |
| ATOM | 3988 | NZ  | LYS | 1106 | 98.374  | 62.649 | 17.655 | 1.00 | 43.75 |
| ATOM | 3989 | C   | LYS | 1106 | 100.485 | 66.760 | 22.465 | 1.00 | 34.26 |
| ATOM | 3990 | O   | LYS | 1106 | 100.459 | 67.946 | 22.128 | 1.00 | 35.05 |
| ATOM | 3991 | N   | VAL | 1107 | 99.808  | 66.293 | 23.510 | 1.00 | 33.42 |
| ATOM | 3992 | CA  | VAL | 1107 | 99.002  | 67.178 | 24.338 | 1.00 | 33.04 |
| ATOM | 3993 | CB  | VAL | 1107 | 97.977  | 66.394 | 25.195 | 1.00 | 29.85 |
| ATOM | 3994 | CG1 | VAL | 1107 | 97.189  | 67.340 | 26.089 | 1.00 | 24.12 |
| ATOM | 3995 | CG2 | VAL | 1107 | 97.031  | 65.624 | 24.302 | 1.00 | 30.73 |
| ATOM | 3996 | C   | VAL | 1107 | 99.920  | 67.967 | 25.258 | 1.00 | 35.29 |
| ATOM | 3997 | O   | VAL | 1107 | 99.868  | 69.196 | 25.300 | 1.00 | 36.49 |
| ATOM | 3998 | N   | LYS | 1108 | 100.793 | 67.258 | 25.959 | 1.00 | 36.76 |
| ATOM | 3999 | CA  | LYS | 1108 | 101.710 | 67.892 | 26.888 | 1.00 | 38.65 |

FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 4000 | CB  | LYS | 1108 | 102.483 | 66.838 | 27.673 | 1.00 | 37.67 |
| ATOM | 4001 | CG  | LYS | 1108 | 101.612 | 66.008 | 28.598 | 1.00 | 36.98 |
| ATOM | 4002 | CD  | LYS | 1108 | 100.862 | 66.881 | 29.597 | 1.00 | 36.47 |
| ATOM | 4003 | CE  | LYS | 1108 | 101.809 | 67.684 | 30.471 | 1.00 | 36.82 |
| ATOM | 4004 | NZ  | LYS | 1108 | 101.090 | 68.507 | 31.484 | 1.00 | 38.27 |
| ATOM | 4005 | C   | LYS | 1108 | 102.663 | 68.859 | 26.208 | 1.00 | 41.58 |
| ATOM | 4006 | O   | LYS | 1108 | 103.097 | 69.835 | 26.821 | 1.00 | 41.70 |
| ATOM | 4007 | N   | LYS | 1109 | 102.970 | 68.598 | 24.939 | 1.00 | 44.26 |
| ATOM | 4008 | CA  | LYS | 1109 | 103.866 | 69.457 | 24.172 | 1.00 | 46.63 |
| ATOM | 4009 | CB  | LYS | 1109 | 104.735 | 68.625 | 23.227 | 1.00 | 48.92 |
| ATOM | 4010 | CG  | LYS | 1109 | 105.765 | 67.752 | 23.925 | 1.00 | 55.10 |
| ATOM | 4011 | CD  | LYS | 1109 | 106.649 | 67.038 | 22.917 | 1.00 | 57.86 |
| ATOM | 4012 | CE  | LYS | 1109 | 107.698 | 66.190 | 23.607 | 1.00 | 60.67 |
| ATOM | 4013 | NZ  | LYS | 1109 | 108.539 | 65.453 | 22.624 | 1.00 | 64.20 |
| ATOM | 4014 | C   | LYS | 1109 | 103.116 | 70.503 | 23.361 | 1.00 | 48.09 |
| ATOM | 4015 | O   | LYS | 1109 | 103.704 | 71.143 | 22.494 | 1.00 | 50.31 |
| ATOM | 4016 | N   | TYR | 1110 | 101.823 | 70.671 | 23.622 | 1.00 | 49.80 |
| ATOM | 4017 | CA  | TYR | 1110 | 101.032 | 71.647 | 22.883 | 1.00 | 50.56 |
| ATOM | 4018 | CB  | TYR | 1110 | 99.526  | 71.410 | 23.054 | 1.00 | 49.06 |
| ATOM | 4019 | CG  | TYR | 1110 | 98.671  | 72.376 | 22.240 | 1.00 | 45.63 |
| ATOM | 4020 | CD1 | TYR | 1110 | 98.377  | 72.117 | 20.902 | 1.00 | 42.22 |
| ATOM | 4021 | CE1 | TYR | 1110 | 97.615  | 73.001 | 20.145 | 1.00 | 39.41 |
| ATOM | 4022 | CD2 | TYR | 1110 | 98.172  | 73.556 | 22.805 | 1.00 | 41.44 |
| ATOM | 4023 | CE2 | TYR | 1110 | 97.410  | 74.449 | 22.053 | 1.00 | 38.41 |
| ATOM | 4024 | CZ  | TYR | 1110 | 97.135  | 74.162 | 20.723 | 1.00 | 39.73 |
| ATOM | 4025 | OH  | TYR | 1110 | 96.377  | 75.028 | 19.969 | 1.00 | 42.38 |
| ATOM | 4026 | C   | TYR | 1110 | 101.338 | 73.080 | 23.262 | 1.00 | 52.16 |
| ATOM | 4027 | O   | TYR | 1110 | 101.405 | 73.433 | 24.436 | 1.00 | 50.66 |
| ATOM | 4028 | N   | GLU | 1111 | 101.470 | 73.909 | 22.238 | 1.00 | 56.35 |
| ATOM | 4029 | CA  | GLU | 1111 | 101.726 | 75.326 | 22.407 | 1.00 | 62.85 |
| ATOM | 4030 | CB  | GLU | 1111 | 103.170 | 75.580 | 22.846 | 1.00 | 68.99 |
| ATOM | 4031 | CG  | GLU | 1111 | 103.473 | 77.039 | 23.221 | 1.00 | 78.92 |
| ATOM | 4032 | CD  | GLU | 1111 | 102.841 | 77.479 | 24.544 | 1.00 | 86.72 |
| ATOM | 4033 | OE1 | GLU | 1111 | 103.602 | 77.833 | 25.476 | 1.00 | 88.71 |
| ATOM | 4034 | OE2 | GLU | 1111 | 101.591 | 77.492 | 24.650 | 1.00 | 89.94 |
| ATOM | 4035 | C   | GLU | 1111 | 101.456 | 75.977 | 21.063 | 1.00 | 64.72 |
| ATOM | 4036 | O   | GLU | 1111 | 102.047 | 75.595 | 20.049 | 1.00 | 64.03 |
| ATOM | 4037 | N   | GLN | 1112 | 100.489 | 76.890 | 21.049 | 1.00 | 67.72 |
| ATOM | 4038 | CA  | GLN | 1112 | 100.103 | 77.616 | 19.842 | 1.00 | 71.20 |
| ATOM | 4039 | CB  | GLN | 1112 | 99.391  | 76.686 | 18.850 | 1.00 | 74.46 |
| ATOM | 4040 | CG  | GLN | 1112 | 99.112  | 77.314 | 17.482 | 1.00 | 77.35 |
| ATOM | 4041 | CD  | GLN | 1112 | 98.260  | 76.426 | 16.589 | 1.00 | 78.90 |
| ATOM | 4042 | OE1 | GLN | 1112 | 97.039  | 76.566 | 16.542 | 1.00 | 79.16 |
| ATOM | 4043 | NE2 | GLN | 1112 | 98.901  | 75.505 | 15.876 | 1.00 | 79.35 |
| ATOM | 4044 | C   | GLN | 1112 | 99.168  | 78.752 | 20.240 | 1.00 | 71.94 |
| ATOM | 4045 | O   | GLN | 1112 | 98.417  | 78.542 | 21.217 | 1.00 | 72.65 |
| ATOM | 4046 | CB  | TYR | 1233 | 92.594  | 79.434 | 26.175 | 1.00 | 39.31 |
| ATOM | 4047 | CG  | TYR | 1233 | 92.140  | 78.944 | 24.817 | 1.00 | 39.59 |
| ATOM | 4048 | CD1 | TYR | 1233 | 90.810  | 78.606 | 24.585 | 1.00 | 39.63 |
| ATOM | 4049 | CE1 | TYR | 1233 | 90.390  | 78.142 | 23.339 | 1.00 | 42.81 |
| ATOM | 4050 | CD2 | TYR | 1233 | 93.045  | 78.808 | 23.766 | 1.00 | 42.38 |
| ATOM | 4051 | CE2 | TYR | 1233 | 92.637  | 78.345 | 22.511 | 1.00 | 42.93 |
| ATOM | 4052 | CZ  | TYR | 1233 | 91.306  | 78.015 | 22.306 | 1.00 | 42.57 |
| ATOM | 4053 | OH  | TYR | 1233 | 90.884  | 77.574 | 21.072 | 1.00 | 41.24 |
| ATOM | 4054 | C   | TYR | 1233 | 92.326  | 81.012 | 28.108 | 1.00 | 34.30 |
| ATOM | 4055 | O   | TYR | 1233 | 93.223  | 80.365 | 28.647 | 1.00 | 35.38 |
| ATOM | 4056 | N   | TYR | 1233 | 92.175  | 81.859 | 25.767 | 1.00 | 37.90 |
| ATOM | 4057 | CA  | TYR | 1233 | 91.886  | 80.707 | 26.674 | 1.00 | 36.86 |

## FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 4058 | N   | PRO | 1234 | 91.675  | 81.987 | 28.757 | 1.00 | 31.05 |
| ATOM | 4059 | CD  | PRO | 1234 | 90.523  | 82.770 | 28.281 | 1.00 | 31.27 |
| ATOM | 4060 | CA  | PRO | 1234 | 92.027  | 82.350 | 30.133 | 1.00 | 28.70 |
| ATOM | 4061 | CB  | PRO | 1234 | 91.180  | 83.594 | 30.376 | 1.00 | 29.55 |
| ATOM | 4062 | CG  | PRO | 1234 | 89.951  | 83.318 | 29.567 | 1.00 | 31.87 |
| ATOM | 4063 | C   | PRO | 1234 | 91.729  | 81.267 | 31.164 | 1.00 | 27.05 |
| ATOM | 4064 | O   | PRO | 1234 | 92.097  | 81.409 | 32.327 | 1.00 | 24.79 |
| ATOM | 4065 | N   | LEU | 1235 | 91.013  | 80.224 | 30.740 | 1.00 | 28.44 |
| ATOM | 4066 | CA  | LEU | 1235 | 90.639  | 79.101 | 31.607 | 1.00 | 27.99 |
| ATOM | 4067 | CB  | LEU | 1235 | 89.174  | 78.715 | 31.406 | 1.00 | 27.25 |
| ATOM | 4068 | CG  | LEU | 1235 | 88.100  | 79.751 | 31.680 | 1.00 | 25.62 |
| ATOM | 4069 | CD1 | LEU | 1235 | 86.739  | 79.084 | 31.530 | 1.00 | 24.42 |
| ATOM | 4070 | CD2 | LEU | 1235 | 88.292  | 80.323 | 33.078 | 1.00 | 26.15 |
| ATOM | 4071 | C   | LEU | 1235 | 91.466  | 77.876 | 31.299 | 1.00 | 28.14 |
| ATOM | 4072 | O   | LEU | 1235 | 91.308  | 76.835 | 31.944 | 1.00 | 25.67 |
| ATOM | 4073 | N   | ALA | 1236 | 92.279  | 77.979 | 30.253 | 1.00 | 29.94 |
| ATOM | 4074 | CA  | ALA | 1236 | 93.130  | 76.884 | 29.843 | 1.00 | 31.57 |
| ATOM | 4075 | CB  | ALA | 1236 | 94.179  | 77.373 | 28.891 | 1.00 | 32.74 |
| ATOM | 4076 | C   | ALA | 1236 | 93.765  | 76.314 | 31.094 | 1.00 | 33.80 |
| ATOM | 4077 | O   | ALA | 1236 | 94.304  | 77.050 | 31.926 | 1.00 | 34.29 |
| ATOM | 4078 | N   | SER | 1237 | 93.574  | 75.020 | 31.288 | 1.00 | 35.41 |
| ATOM | 4079 | CA  | SER | 1237 | 94.118  | 74.352 | 32.445 | 1.00 | 39.00 |
| ATOM | 4080 | CB  | SER | 1237 | 93.041  | 73.452 | 33.068 | 1.00 | 42.92 |
| ATOM | 4081 | OG  | SER | 1237 | 91.989  | 74.237 | 33.636 | 1.00 | 43.86 |
| ATOM | 4082 | C   | SER | 1237 | 95.401  | 73.599 | 32.085 | 1.00 | 39.38 |
| ATOM | 4083 | O   | SER | 1237 | 95.403  | 72.668 | 31.270 | 1.00 | 39.77 |
| ATOM | 4084 | N   | LYS | 1238 | 96.507  | 74.064 | 32.656 | 1.00 | 39.71 |
| ATOM | 4085 | CA  | LYS | 1238 | 97.813  | 73.474 | 32.413 | 1.00 | 41.61 |
| ATOM | 4086 | CB  | LYS | 1238 | 98.587  | 74.304 | 31.382 | 1.00 | 43.64 |
| ATOM | 4087 | CG  | LYS | 1238 | 98.336  | 75.804 | 31.401 | 1.00 | 46.63 |
| ATOM | 4088 | CD  | LYS | 1238 | 98.532  | 76.385 | 29.993 | 1.00 | 49.43 |
| ATOM | 4089 | CE  | LYS | 1238 | 98.469  | 77.915 | 29.954 | 1.00 | 52.17 |
| ATOM | 4090 | NZ  | LYS | 1238 | 97.166  | 78.480 | 30.418 | 1.00 | 53.93 |
| ATOM | 4091 | C   | LYS | 1238 | 98.611  | 73.306 | 33.697 | 1.00 | 41.85 |
| ATOM | 4092 | O   | LYS | 1238 | 98.215  | 73.815 | 34.745 | 1.00 | 42.33 |
| ATOM | 4093 | N   | ASP | 1239 | 99.695  | 72.538 | 33.627 | 1.00 | 42.02 |
| ATOM | 4094 | CA  | ASP | 1239 | 100.541 | 72.289 | 34.788 | 1.00 | 43.25 |
| ATOM | 4095 | CB  | ASP | 1239 | 101.277 | 70.950 | 34.637 | 1.00 | 42.65 |
| ATOM | 4096 | CG  | ASP | 1239 | 102.252 | 70.933 | 33.470 | 1.00 | 41.63 |
| ATOM | 4097 | OD1 | ASP | 1239 | 102.274 | 71.902 | 32.694 | 1.00 | 43.12 |
| ATOM | 4098 | OD2 | ASP | 1239 | 103.007 | 69.946 | 33.328 | 1.00 | 41.56 |
| ATOM | 4099 | C   | ASP | 1239 | 101.534 | 73.416 | 35.085 | 1.00 | 45.87 |
| ATOM | 4100 | O   | ASP | 1239 | 101.579 | 74.430 | 34.381 | 1.00 | 46.72 |
| ATOM | 4101 | N   | ALA | 1240 | 102.364 | 73.196 | 36.104 | 1.00 | 46.78 |
| ATOM | 4102 | CA  | ALA | 1240 | 103.370 | 74.162 | 36.548 | 1.00 | 46.30 |
| ATOM | 4103 | CB  | ALA | 1240 | 104.203 | 73.562 | 37.676 | 1.00 | 46.81 |
| ATOM | 4104 | C   | ALA | 1240 | 104.282 | 74.683 | 35.439 | 1.00 | 45.64 |
| ATOM | 4105 | O   | ALA | 1240 | 104.675 | 75.851 | 35.446 | 1.00 | 46.51 |
| ATOM | 4106 | N   | LYS | 1241 | 104.628 | 73.816 | 34.495 | 1.00 | 43.50 |
| ATOM | 4107 | CA  | LYS | 1241 | 105.486 | 74.216 | 33.391 | 1.00 | 41.50 |
| ATOM | 4108 | CB  | LYS | 1241 | 106.327 | 73.028 | 32.927 | 1.00 | 42.33 |
| ATOM | 4109 | CG  | LYS | 1241 | 107.198 | 72.458 | 34.040 | 1.00 | 45.75 |
| ATOM | 4110 | CD  | LYS | 1241 | 108.136 | 71.364 | 33.549 | 1.00 | 52.02 |
| ATOM | 4111 | CE  | LYS | 1241 | 107.394 | 70.096 | 33.147 | 1.00 | 56.80 |
| ATOM | 4112 | NZ  | LYS | 1241 | 108.330 | 69.053 | 32.625 | 1.00 | 59.79 |
| ATOM | 4113 | C   | LYS | 1241 | 104.668 | 74.808 | 32.246 | 1.00 | 40.64 |
| ATOM | 4114 | O   | LYS | 1241 | 105.119 | 74.850 | 31.102 | 1.00 | 39.48 |
| ATOM | 4115 | N   | LYS | 1242 | 103.451 | 75.244 | 32.575 | 1.00 | 40.74 |

FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 4116 | CA  | LYS | 1242 | 102.525 | 75.863 | 31.635 | 1.00 | 40.98 |
| ATOM | 4117 | CB  | LYS | 1242 | 103.130 | 77.162 | 31.102 | 1.00 | 46.48 |
| ATOM | 4118 | CG  | LYS | 1242 | 103.655 | 78.106 | 32.184 | 1.00 | 54.66 |
| ATOM | 4119 | CD  | LYS | 1242 | 104.504 | 79.227 | 31.567 | 1.00 | 63.33 |
| ATOM | 4120 | CE  | LYS | 1242 | 105.116 | 80.153 | 32.623 | 1.00 | 68.01 |
| ATOM | 4121 | NZ  | LYS | 1242 | 106.121 | 79.459 | 33.488 | 1.00 | 71.11 |
| ATOM | 4122 | C   | LYS | 1242 | 102.068 | 74.977 | 30.471 | 1.00 | 40.38 |
| ATOM | 4123 | O   | LYS | 1242 | 101.545 | 75.471 | 29.472 | 1.00 | 40.63 |
| ATOM | 4124 | N   | GLN | 1243 | 102.281 | 73.672 | 30.582 | 1.00 | 38.45 |
| ATOM | 4125 | CA  | GLN | 1243 | 101.863 | 72.749 | 29.531 | 1.00 | 37.94 |
| ATOM | 4126 | CB  | GLN | 1243 | 102.905 | 71.640 | 29.338 | 1.00 | 42.14 |
| ATOM | 4127 | CG  | GLN | 1243 | 104.293 | 72.126 | 28.894 | 1.00 | 50.87 |
| ATOM | 4128 | CD  | GLN | 1243 | 104.296 | 72.805 | 27.516 | 1.00 | 58.97 |
| ATOM | 4129 | OE1 | GLN | 1243 | 104.790 | 72.248 | 26.533 | 1.00 | 61.73 |
| ATOM | 4130 | NE2 | GLN | 1243 | 103.777 | 74.026 | 27.454 | 1.00 | 61.92 |
| ATOM | 4131 | C   | GLN | 1243 | 100.502 | 72.162 | 29.907 | 1.00 | 35.65 |
| ATOM | 4132 | O   | GLN | 1243 | 100.286 | 71.781 | 31.059 | 1.00 | 34.91 |
| ATOM | 4133 | N   | LEU | 1244 | 99.577  | 72.130 | 28.949 | 1.00 | 33.29 |
| ATOM | 4134 | CA  | LEU | 1244 | 98.221  | 71.614 | 29.176 | 1.00 | 29.46 |
| ATOM | 4135 | CB  | LEU | 1244 | 97.495  | 71.389 | 27.848 | 1.00 | 27.97 |
| ATOM | 4136 | CG  | LEU | 1244 | 97.232  | 72.570 | 26.922 | 1.00 | 25.53 |
| ATOM | 4137 | CD1 | LEU | 1244 | 96.497  | 72.069 | 25.701 | 1.00 | 23.64 |
| ATOM | 4138 | CD2 | LEU | 1244 | 96.426  | 73.639 | 27.631 | 1.00 | 26.68 |
| ATOM | 4139 | C   | LEU | 1244 | 98.174  | 70.315 | 29.964 | 1.00 | 26.37 |
| ATOM | 4140 | O   | LEU | 1244 | 98.990  | 69.423 | 29.759 | 1.00 | 25.40 |
| ATOM | 4141 | N   | LEU | 1245 | 97.203  | 70.208 | 30.861 | 1.00 | 24.19 |
| ATOM | 4142 | CA  | LEU | 1245 | 97.043  | 69.000 | 31.654 | 1.00 | 21.24 |
| ATOM | 4143 | CB  | LEU | 1245 | 96.010  | 69.226 | 32.750 | 1.00 | 17.87 |
| ATOM | 4144 | CG  | LEU | 1245 | 96.388  | 70.166 | 33.886 | 1.00 | 13.30 |
| ATOM | 4145 | CD1 | LEU | 1245 | 95.278  | 70.190 | 34.957 | 1.00 | 8.28  |
| ATOM | 4146 | CD2 | LEU | 1245 | 97.692  | 69.691 | 34.476 | 1.00 | 12.89 |
| ATOM | 4147 | C   | LEU | 1245 | 96.577  | 67.851 | 30.760 | 1.00 | 22.73 |
| ATOM | 4148 | O   | LEU | 1245 | 95.875  | 68.067 | 29.772 | 1.00 | 22.07 |
| ATOM | 4149 | N   | CYS | 1246 | 96.970  | 66.631 | 31.097 | 1.00 | 23.09 |
| ATOM | 4150 | CA  | CYS | 1246 | 96.561  | 65.481 | 30.311 | 1.00 | 24.22 |
| ATOM | 4151 | CB  | CYS | 1246 | 97.564  | 65.167 | 29.213 | 1.00 | 23.07 |
| ATOM | 4152 | SG  | CYS | 1246 | 96.980  | 63.858 | 28.114 | 1.00 | 28.22 |
| ATOM | 4153 | C   | CYS | 1246 | 96.409  | 64.271 | 31.199 | 1.00 | 25.46 |
| ATOM | 4154 | O   | CYS | 1246 | 97.177  | 64.087 | 32.149 | 1.00 | 26.61 |
| ATOM | 4155 | N   | GLY | 1247 | 95.405  | 63.457 | 30.899 | 1.00 | 24.77 |
| ATOM | 4156 | CA  | GLY | 1247 | 95.159  | 62.257 | 31.669 | 1.00 | 23.54 |
| ATOM | 4157 | C   | GLY | 1247 | 95.056  | 61.081 | 30.724 | 1.00 | 22.83 |
| ATOM | 4158 | O   | GLY | 1247 | 94.823  | 61.260 | 29.525 | 1.00 | 22.59 |
| ATOM | 4159 | N   | ALA | 1248 | 95.230  | 59.878 | 31.252 | 1.00 | 20.75 |
| ATOM | 4160 | CA  | ALA | 1248 | 95.150  | 58.678 | 30.437 | 1.00 | 20.33 |
| ATOM | 4161 | CB  | ALA | 1248 | 96.536  | 58.256 | 29.990 | 1.00 | 21.90 |
| ATOM | 4162 | C   | ALA | 1248 | 94.485  | 57.561 | 31.222 | 1.00 | 20.51 |
| ATOM | 4163 | O   | ALA | 1248 | 94.619  | 57.473 | 32.447 | 1.00 | 18.34 |
| ATOM | 4164 | N   | ALA | 1249 | 93.740  | 56.727 | 30.514 | 1.00 | 20.76 |
| ATOM | 4165 | CA  | ALA | 1249 | 93.050  | 55.622 | 31.140 | 1.00 | 22.52 |
| ATOM | 4166 | CB  | ALA | 1249 | 91.670  | 55.477 | 30.543 | 1.00 | 22.47 |
| ATOM | 4167 | C   | ALA | 1249 | 93.825  | 54.342 | 30.928 | 1.00 | 24.15 |
| ATOM | 4168 | O   | ALA | 1249 | 94.183  | 54.019 | 29.790 | 1.00 | 25.00 |
| ATOM | 4169 | N   | ILE | 1250 | 94.105  | 53.616 | 32.005 | 1.00 | 23.49 |
| ATOM | 4170 | CA  | ILE | 1250 | 94.794  | 52.341 | 31.860 | 1.00 | 24.48 |
| ATOM | 4171 | CB  | ILE | 1250 | 96.254  | 52.330 | 32.417 | 1.00 | 22.98 |
| ATOM | 4172 | CG2 | ILE | 1250 | 97.088  | 53.412 | 31.760 | 1.00 | 24.80 |
| ATOM | 4173 | CG1 | ILE | 1250 | 96.276  | 52.433 | 33.939 | 1.00 | 20.21 |



FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 4174 | CD1 | ILE | 1250 | 97.629  | 52.107 | 34.530 | 1.00 | 18.03 |
| ATOM | 4175 | C   | ILE | 1250 | 93.999  | 51.227 | 32.520 | 1.00 | 25.11 |
| ATOM | 4176 | O   | ILE | 1250 | 93.044  | 51.476 | 33.253 | 1.00 | 21.56 |
| ATOM | 4177 | N   | GLY | 1251 | 94.337  | 49.998 | 32.156 | 1.00 | 29.40 |
| ATOM | 4178 | CA  | GLY | 1251 | 93.693  | 48.842 | 32.740 | 1.00 | 32.82 |
| ATOM | 4179 | C   | GLY | 1251 | 94.479  | 48.532 | 33.996 | 1.00 | 36.17 |
| ATOM | 4180 | O   | GLY | 1251 | 95.271  | 49.350 | 34.451 | 1.00 | 38.38 |
| ATOM | 4181 | N   | THR | 1252 | 94.345  | 47.326 | 34.513 | 1.00 | 39.63 |
| ATOM | 4182 | CA  | THR | 1252 | 95.060  | 46.990 | 35.725 | 1.00 | 43.76 |
| ATOM | 4183 | CB  | THR | 1252 | 94.057  | 46.575 | 36.818 | 1.00 | 41.72 |
| ATOM | 4184 | OG1 | THR | 1252 | 93.203  | 47.687 | 37.124 | 1.00 | 37.90 |
| ATOM | 4185 | CG2 | THR | 1252 | 94.771  | 46.155 | 38.066 | 1.00 | 47.51 |
| ATOM | 4186 | C   | THR | 1252 | 96.179  | 45.956 | 35.538 | 1.00 | 48.10 |
| ATOM | 4187 | O   | THR | 1252 | 97.349  | 46.256 | 35.772 | 1.00 | 48.88 |
| ATOM | 4188 | N   | HIS | 1253 | 95.825  | 44.772 | 35.047 | 1.00 | 51.97 |
| ATOM | 4189 | CA  | HIS | 1253 | 96.790  | 43.689 | 34.844 | 1.00 | 56.55 |
| ATOM | 4190 | CB  | HIS | 1253 | 96.197  | 42.583 | 33.956 | 1.00 | 63.58 |
| ATOM | 4191 | CG  | HIS | 1253 | 95.708  | 43.060 | 32.625 | 1.00 | 71.59 |
| ATOM | 4192 | CD2 | HIS | 1253 | 94.873  | 44.069 | 32.288 | 1.00 | 76.45 |
| ATOM | 4193 | ND1 | HIS | 1253 | 96.072  | 42.451 | 31.439 | 1.00 | 77.55 |
| ATOM | 4194 | CE1 | HIS | 1253 | 95.480  | 43.071 | 30.431 | 1.00 | 81.02 |
| ATOM | 4195 | NE2 | HIS | 1253 | 94.749  | 44.055 | 30.917 | 1.00 | 80.91 |
| ATOM | 4196 | C   | HIS | 1253 | 98.173  | 44.083 | 34.334 | 1.00 | 56.12 |
| ATOM | 4197 | O   | HIS | 1253 | 98.295  | 44.864 | 33.398 | 1.00 | 56.78 |
| ATOM | 4198 | N   | GLU | 1254 | 99.191  | 43.495 | 34.963 | 1.00 | 56.64 |
| ATOM | 4199 | CA  | GLU | 1254 | 100.617 | 43.690 | 34.672 | 1.00 | 56.02 |
| ATOM | 4200 | CB  | GLU | 1254 | 101.309 | 42.329 | 34.570 | 1.00 | 57.76 |
| ATOM | 4201 | CG  | GLU | 1254 | 101.379 | 41.554 | 35.879 | 1.00 | 61.36 |
| ATOM | 4202 | CD  | GLU | 1254 | 102.378 | 42.136 | 36.867 | 1.00 | 64.92 |
| ATOM | 4203 | OE1 | GLU | 1254 | 103.524 | 42.443 | 36.458 | 1.00 | 64.68 |
| ATOM | 4204 | OE2 | GLU | 1254 | 102.016 | 42.270 | 38.058 | 1.00 | 66.93 |
| ATOM | 4205 | C   | GLU | 1254 | 101.009 | 44.525 | 33.462 | 1.00 | 53.65 |
| ATOM | 4206 | O   | GLU | 1254 | 101.767 | 45.480 | 33.582 | 1.00 | 53.34 |
| ATOM | 4207 | N   | ASP | 1255 | 100.532 | 44.113 | 32.294 | 1.00 | 52.31 |
| ATOM | 4208 | CA  | ASP | 1255 | 100.803 | 44.782 | 31.024 | 1.00 | 50.29 |
| ATOM | 4209 | CB  | ASP | 1255 | 99.804  | 44.290 | 29.973 | 1.00 | 55.04 |
| ATOM | 4210 | CG  | ASP | 1255 | 99.626  | 42.775 | 29.993 | 1.00 | 61.28 |
| ATOM | 4211 | OD1 | ASP | 1255 | 98.900  | 42.259 | 30.881 | 1.00 | 59.30 |
| ATOM | 4212 | OD2 | ASP | 1255 | 100.220 | 42.105 | 29.118 | 1.00 | 65.78 |
| ATOM | 4213 | C   | ASP | 1255 | 100.695 | 46.301 | 31.129 | 1.00 | 47.04 |
| ATOM | 4214 | O   | ASP | 1255 | 101.447 | 47.039 | 30.490 | 1.00 | 46.57 |
| ATOM | 4215 | N   | ASP | 1256 | 99.768  | 46.752 | 31.967 | 1.00 | 44.52 |
| ATOM | 4216 | CA  | ASP | 1256 | 99.501  | 48.173 | 32.171 | 1.00 | 41.04 |
| ATOM | 4217 | CB  | ASP | 1256 | 98.142  | 48.352 | 32.847 | 1.00 | 39.06 |
| ATOM | 4218 | CG  | ASP | 1256 | 97.012  | 47.813 | 32.003 | 1.00 | 36.49 |
| ATOM | 4219 | OD1 | ASP | 1256 | 96.720  | 48.422 | 30.955 | 1.00 | 32.75 |
| ATOM | 4220 | OD2 | ASP | 1256 | 96.432  | 46.769 | 32.368 | 1.00 | 37.91 |
| ATOM | 4221 | C   | ASP | 1256 | 100.584 | 48.924 | 32.920 | 1.00 | 37.97 |
| ATOM | 4222 | O   | ASP | 1256 | 100.585 | 50.153 | 32.945 | 1.00 | 35.60 |
| ATOM | 4223 | N   | LYS | 1257 | 101.505 | 48.180 | 33.520 | 1.00 | 37.65 |
| ATOM | 4224 | CA  | LYS | 1257 | 102.619 | 48.765 | 34.253 | 1.00 | 36.92 |
| ATOM | 4225 | CB  | LYS | 1257 | 103.325 | 47.693 | 35.078 | 1.00 | 36.40 |
| ATOM | 4226 | CG  | LYS | 1257 | 102.465 | 47.092 | 36.172 | 1.00 | 37.53 |
| ATOM | 4227 | CD  | LYS | 1257 | 103.251 | 46.074 | 36.978 | 1.00 | 41.41 |
| ATOM | 4228 | CE  | LYS | 1257 | 102.581 | 45.760 | 38.309 | 1.00 | 43.29 |
| ATOM | 4229 | NZ  | LYS | 1257 | 101.232 | 45.166 | 38.132 | 1.00 | 47.58 |
| ATOM | 4230 | C   | LYS | 1257 | 103.590 | 49.406 | 33.258 | 1.00 | 36.36 |
| ATOM | 4231 | O   | LYS | 1257 | 104.009 | 50.554 | 33.431 | 1.00 | 34.55 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3768 | N   | GLY | 1077 | 93.480 | 65.613 | 20.144 | 1.00 | 34.10 |
| ATOM | 3769 | CA  | GLY | 1077 | 92.655 | 66.763 | 19.810 | 1.00 | 34.49 |
| ATOM | 3770 | C   | GLY | 1077 | 91.655 | 67.146 | 20.886 | 1.00 | 35.44 |
| ATOM | 3771 | O   | GLY | 1077 | 91.574 | 68.314 | 21.278 | 1.00 | 35.30 |
| ATOM | 3772 | N   | MET | 1078 | 90.895 | 66.159 | 21.356 | 1.00 | 35.00 |
| ATOM | 3773 | CA  | MET | 1078 | 89.892 | 66.361 | 22.400 | 1.00 | 32.60 |
| ATOM | 3774 | CB  | MET | 1078 | 89.122 | 65.060 | 22.650 | 1.00 | 30.21 |
| ATOM | 3775 | CG  | MET | 1078 | 88.115 | 65.119 | 23.787 | 1.00 | 23.97 |
| ATOM | 3776 | SD  | MET | 1078 | 86.729 | 66.180 | 23.420 | 1.00 | 22.65 |
| ATOM | 3777 | CE  | MET | 1078 | 85.882 | 65.186 | 22.153 | 1.00 | 13.83 |
| ATOM | 3778 | C   | MET | 1078 | 90.562 | 66.806 | 23.691 | 1.00 | 32.54 |
| ATOM | 3779 | O   | MET | 1078 | 90.281 | 67.890 | 24.205 | 1.00 | 33.25 |
| ATOM | 3780 | N   | ALA | 1079 | 91.473 | 65.975 | 24.191 | 1.00 | 29.80 |
| ATOM | 3781 | CA  | ALA | 1079 | 92.185 | 66.264 | 25.426 | 1.00 | 26.90 |
| ATOM | 3782 | CB  | ALA | 1079 | 93.312 | 65.272 | 25.625 | 1.00 | 25.36 |
| ATOM | 3783 | C   | ALA | 1079 | 92.719 | 67.686 | 25.411 | 1.00 | 26.03 |
| ATOM | 3784 | O   | ALA | 1079 | 92.675 | 68.385 | 26.426 | 1.00 | 25.26 |
| ATOM | 3785 | N   | ILE | 1080 | 93.163 | 68.132 | 24.238 | 1.00 | 26.03 |
| ATOM | 3786 | CA  | ILE | 1080 | 93.696 | 69.481 | 24.082 | 1.00 | 25.73 |
| ATOM | 3787 | CB  | ILE | 1080 | 94.486 | 69.632 | 22.761 | 1.00 | 23.56 |
| ATOM | 3788 | CG2 | ILE | 1080 | 94.898 | 71.086 | 22.540 | 1.00 | 22.24 |
| ATOM | 3789 | CG1 | ILE | 1080 | 95.740 | 68.763 | 22.810 | 1.00 | 21.45 |
| ATOM | 3790 | CD1 | ILE | 1080 | 96.565 | 68.809 | 21.554 | 1.00 | 22.68 |
| ATOM | 3791 | C   | ILE | 1080 | 92.587 | 70.530 | 24.154 | 1.00 | 26.48 |
| ATOM | 3792 | O   | ILE | 1080 | 92.645 | 71.444 | 24.979 | 1.00 | 25.96 |
| ATOM | 3793 | N   | ALA | 1081 | 91.559 | 70.369 | 23.323 | 1.00 | 27.21 |
| ATOM | 3794 | CA  | ALA | 1081 | 90.438 | 71.305 | 23.285 | 1.00 | 25.13 |
| ATOM | 3795 | CB  | ALA | 1081 | 89.422 | 70.866 | 22.240 | 1.00 | 23.36 |
| ATOM | 3796 | C   | ALA | 1081 | 89.778 | 71.410 | 24.652 | 1.00 | 25.14 |
| ATOM | 3797 | O   | ALA | 1081 | 89.335 | 72.484 | 25.064 | 1.00 | 26.40 |
| ATOM | 3798 | N   | MET | 1082 | 89.762 | 70.295 | 25.369 | 1.00 | 25.59 |
| ATOM | 3799 | CA  | MET | 1082 | 89.162 | 70.232 | 26.691 | 1.00 | 26.26 |
| ATOM | 3800 | CB  | MET | 1082 | 89.051 | 68.771 | 27.146 | 1.00 | 27.01 |
| ATOM | 3801 | CG  | MET | 1082 | 87.856 | 68.464 | 28.048 | 1.00 | 28.65 |
| ATOM | 3802 | SD  | MET | 1082 | 86.249 | 68.526 | 27.203 | 1.00 | 26.79 |
| ATOM | 3803 | CE  | MET | 1082 | 85.315 | 69.478 | 28.353 | 1.00 | 23.90 |
| ATOM | 3804 | C   | MET | 1082 | 89.992 | 71.056 | 27.675 | 1.00 | 25.81 |
| ATOM | 3805 | O   | MET | 1082 | 89.442 | 71.851 | 28.434 | 1.00 | 26.89 |
| ATOM | 3806 | N   | ALA | 1083 | 91.314 | 70.913 | 27.624 | 1.00 | 25.36 |
| ATOM | 3807 | CA  | ALA | 1083 | 92.195 | 71.663 | 28.519 | 1.00 | 23.07 |
| ATOM | 3808 | CB  | ALA | 1083 | 93.594 | 71.105 | 28.472 | 1.00 | 19.47 |
| ATOM | 3809 | C   | ALA | 1083 | 92.217 | 73.158 | 28.205 | 1.00 | 24.00 |
| ATOM | 3810 | O   | ALA | 1083 | 92.330 | 73.990 | 29.107 | 1.00 | 23.89 |
| ATOM | 3811 | N   | LEU | 1084 | 92.117 | 73.508 | 26.927 | 1.00 | 24.04 |
| ATOM | 3812 | CA  | LEU | 1084 | 92.133 | 74.913 | 26.550 | 1.00 | 21.88 |
| ATOM | 3813 | CB  | LEU | 1084 | 92.278 | 75.092 | 25.031 | 1.00 | 20.51 |
| ATOM | 3814 | CG  | LEU | 1084 | 93.621 | 74.803 | 24.333 | 1.00 | 17.98 |
| ATOM | 3815 | CD1 | LEU | 1084 | 93.489 | 75.021 | 22.834 | 1.00 | 10.91 |
| ATOM | 3816 | CD2 | LEU | 1084 | 94.728 | 75.687 | 24.892 | 1.00 | 16.24 |
| ATOM | 3817 | C   | LEU | 1084 | 90.872 | 75.603 | 27.038 | 1.00 | 23.28 |
| ATOM | 3818 | O   | LEU | 1084 | 90.939 | 76.749 | 27.472 | 1.00 | 24.38 |
| ATOM | 3819 | N   | THR | 1085 | 89.738 | 74.897 | 27.009 | 1.00 | 23.36 |
| ATOM | 3820 | CA  | THR | 1085 | 88.458 | 75.477 | 27.433 | 1.00 | 22.95 |
| ATOM | 3821 | CB  | THR | 1085 | 87.267 | 74.937 | 26.604 | 1.00 | 20.99 |
| ATOM | 3822 | OG1 | THR | 1085 | 87.256 | 73.508 | 26.631 | 1.00 | 25.05 |
| ATOM | 3823 | CG2 | THR | 1085 | 87.370 | 75.410 | 25.176 | 1.00 | 16.76 |
| ATOM | 3824 | C   | THR | 1085 | 88.117 | 75.425 | 28.921 | 1.00 | 23.92 |
| ATOM | 3825 | O   | THR | 1085 | 87.077 | 75.954 | 29.342 | 1.00 | 25.16 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 3826 | N   | GLY | 1086 | 88.973 | 74.791 | 29.716 | 1.00 | 24.85 |
| ATOM | 3827 | CA  | GLY | 1086 | 88.731 | 74.748 | 31.150 | 1.00 | 26.30 |
| ATOM | 3828 | C   | GLY | 1086 | 88.614 | 73.400 | 31.835 | 1.00 | 25.84 |
| ATOM | 3829 | O   | GLY | 1086 | 88.517 | 73.336 | 33.063 | 1.00 | 26.47 |
| ATOM | 3830 | N   | GLY | 1087 | 88.570 | 72.332 | 31.057 | 1.00 | 25.34 |
| ATOM | 3831 | CA  | GLY | 1087 | 88.464 | 71.013 | 31.641 | 1.00 | 24.99 |
| ATOM | 3832 | C   | GLY | 1087 | 89.723 | 70.212 | 31.406 | 1.00 | 24.03 |
| ATOM | 3833 | O   | GLY | 1087 | 90.823 | 70.761 | 31.358 | 1.00 | 23.72 |
| ATOM | 3834 | N   | ILE | 1088 | 89.555 | 68.908 | 31.244 | 1.00 | 23.71 |
| ATOM | 3835 | CA  | ILE | 1088 | 90.673 | 68.007 | 31.006 | 1.00 | 23.17 |
| ATOM | 3836 | CB  | ILE | 1088 | 91.360 | 67.582 | 32.352 | 1.00 | 20.71 |
| ATOM | 3837 | CG2 | ILE | 1088 | 90.444 | 66.669 | 33.153 | 1.00 | 20.78 |
| ATOM | 3838 | CG1 | ILE | 1088 | 92.706 | 66.886 | 32.090 | 1.00 | 17.22 |
| ATOM | 3839 | CD1 | ILE | 1088 | 93.545 | 66.593 | 33.353 | 1.00 | 5.96  |
| ATOM | 3840 | C   | ILE | 1088 | 90.083 | 66.799 | 30.283 | 1.00 | 22.59 |
| ATOM | 3841 | O   | ILE | 1088 | 88.862 | 66.605 | 30.281 | 1.00 | 22.13 |
| ATOM | 3842 | N   | GLY | 1089 | 90.939 | 66.023 | 29.630 | 1.00 | 22.64 |
| ATOM | 3843 | CA  | GLY | 1089 | 90.476 | 64.853 | 28.912 | 1.00 | 21.60 |
| ATOM | 3844 | C   | GLY | 1089 | 91.292 | 63.622 | 29.250 | 1.00 | 22.41 |
| ATOM | 3845 | O   | GLY | 1089 | 92.433 | 63.728 | 29.697 | 1.00 | 22.07 |
| ATOM | 3846 | N   | PHE | 1090 | 90.702 | 62.449 | 29.068 | 1.00 | 22.64 |
| ATOM | 3847 | CA  | PHE | 1090 | 91.403 | 61.215 | 29.350 | 1.00 | 22.39 |
| ATOM | 3848 | CB  | PHE | 1090 | 90.668 | 60.425 | 30.423 | 1.00 | 24.55 |
| ATOM | 3849 | CG  | PHE | 1090 | 90.775 | 61.026 | 31.782 | 1.00 | 27.69 |
| ATOM | 3850 | CD1 | PHE | 1090 | 89.903 | 62.032 | 32.181 | 1.00 | 28.68 |
| ATOM | 3851 | CD2 | PHE | 1090 | 91.775 | 60.616 | 32.658 | 1.00 | 26.87 |
| ATOM | 3852 | CE1 | PHE | 1090 | 90.034 | 62.628 | 33.439 | 1.00 | 29.16 |
| ATOM | 3853 | CE2 | PHE | 1090 | 91.912 | 61.207 | 33.917 | 1.00 | 26.20 |
| ATOM | 3854 | CZ  | PHE | 1090 | 91.041 | 62.214 | 34.304 | 1.00 | 29.93 |
| ATOM | 3855 | C   | PHE | 1090 | 91.568 | 60.380 | 28.096 | 1.00 | 22.82 |
| ATOM | 3856 | O   | PHE | 1090 | 90.579 | 59.940 | 27.511 | 1.00 | 23.69 |
| ATOM | 3857 | N   | ILE | 1091 | 92.816 | 60.191 | 27.668 | 1.00 | 21.96 |
| ATOM | 3858 | CA  | ILE | 1091 | 93.114 | 59.394 | 26.480 | 1.00 | 20.77 |
| ATOM | 3859 | CB  | ILE | 1091 | 94.633 | 59.423 | 26.128 | 1.00 | 19.10 |
| ATOM | 3860 | CG2 | ILE | 1091 | 94.892 | 58.635 | 24.846 | 1.00 | 15.49 |
| ATOM | 3861 | CG1 | ILE | 1091 | 95.147 | 60.867 | 25.999 | 1.00 | 13.00 |
| ATOM | 3862 | CD1 | ILE | 1091 | 94.662 | 61.607 | 24.779 | 1.00 | 9.34  |
| ATOM | 3863 | C   | ILE | 1091 | 92.722 | 57.950 | 26.795 | 1.00 | 20.88 |
| ATOM | 3864 | O   | ILE | 1091 | 92.958 | 57.464 | 27.907 | 1.00 | 21.15 |
| ATOM | 3865 | N   | HIS | 1092 | 92.101 | 57.276 | 25.832 | 1.00 | 21.96 |
| ATOM | 3866 | CA  | HIS | 1092 | 91.686 | 55.882 | 26.019 | 1.00 | 23.97 |
| ATOM | 3867 | CB  | HIS | 1092 | 90.613 | 55.492 | 24.994 | 1.00 | 23.05 |
| ATOM | 3868 | CG  | HIS | 1092 | 91.114 | 55.427 | 23.584 | 1.00 | 18.52 |
| ATOM | 3869 | CD2 | HIS | 1092 | 91.563 | 54.381 | 22.849 | 1.00 | 13.17 |
| ATOM | 3870 | ND1 | HIS | 1092 | 91.196 | 56.534 | 22.768 | 1.00 | 15.63 |
| ATOM | 3871 | CE1 | HIS | 1092 | 91.672 | 56.173 | 21.592 | 1.00 | 14.27 |
| ATOM | 3872 | NE2 | HIS | 1092 | 91.908 | 54.873 | 21.614 | 1.00 | 12.20 |
| ATOM | 3873 | C   | HIS | 1092 | 92.887 | 54.946 | 25.895 | 1.00 | 25.60 |
| ATOM | 3874 | O   | HIS | 1092 | 93.957 | 55.369 | 25.467 | 1.00 | 28.13 |
| ATOM | 3875 | N   | HIS | 1093 | 92.708 | 53.675 | 26.242 | 1.00 | 26.03 |
| ATOM | 3876 | CA  | HIS | 1093 | 93.805 | 52.715 | 26.139 | 1.00 | 27.95 |
| ATOM | 3877 | CB  | HIS | 1093 | 94.247 | 52.205 | 27.515 | 1.00 | 29.78 |
| ATOM | 3878 | CG  | HIS | 1093 | 93.231 | 51.358 | 28.218 | 1.00 | 33.05 |
| ATOM | 3879 | CD2 | HIS | 1093 | 93.243 | 50.043 | 28.548 | 1.00 | 34.27 |
| ATOM | 3880 | ND1 | HIS | 1093 | 92.056 | 51.867 | 28.728 | 1.00 | 33.28 |
| ATOM | 3881 | CE1 | HIS | 1093 | 91.388 | 50.906 | 29.338 | 1.00 | 32.87 |
| ATOM | 3882 | NE2 | HIS | 1093 | 92.088 | 49.790 | 29.245 | 1.00 | 34.75 |
| ATOM | 3883 | C   | HIS | 1093 | 93.518 | 51.557 | 25.193 | 1.00 | 28.37 |

FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 3884 | O   | HIS | 1093 | 94.052  | 50.467 | 25.351 | 1.00 | 26.48 |
| ATOM | 3885 | N   | ASN | 1094 | 92.596  | 51.785 | 24.265 | 1.00 | 30.84 |
| ATOM | 3886 | CA  | ASN | 1094 | 92.241  | 50.807 | 23.237 | 1.00 | 32.45 |
| ATOM | 3887 | CB  | ASN | 1094 | 90.769  | 50.963 | 22.842 | 1.00 | 35.56 |
| ATOM | 3888 | CG  | ASN | 1094 | 90.371  | 50.081 | 21.671 | 1.00 | 39.33 |
| ATOM | 3889 | OD1 | ASN | 1094 | 89.850  | 50.568 | 20.668 | 1.00 | 43.29 |
| ATOM | 3890 | ND2 | ASN | 1094 | 90.594  | 48.780 | 21.800 | 1.00 | 38.01 |
| ATOM | 3891 | C   | ASN | 1094 | 93.158  | 51.228 | 22.090 | 1.00 | 33.74 |
| ATOM | 3892 | O   | ASN | 1094 | 92.722  | 51.794 | 21.079 | 1.00 | 34.48 |
| ATOM | 3893 | N   | CYS | 1095 | 94.451  | 51.061 | 22.345 | 1.00 | 33.96 |
| ATOM | 3894 | CA  | CYS | 1095 | 95.517  | 51.431 | 21.427 | 1.00 | 32.91 |
| ATOM | 3895 | CB  | CYS | 1095 | 95.534  | 52.950 | 21.271 | 1.00 | 31.80 |
| ATOM | 3896 | SG  | CYS | 1095 | 95.537  | 53.866 | 22.840 | 1.00 | 33.34 |
| ATOM | 3897 | C   | CYS | 1095 | 96.829  | 50.961 | 22.057 | 1.00 | 33.35 |
| ATOM | 3898 | O   | CYS | 1095 | 96.876  | 50.692 | 23.257 | 1.00 | 34.13 |
| ATOM | 3899 | N   | THR | 1096 | 97.889  | 50.860 | 21.257 | 1.00 | 32.75 |
| ATOM | 3900 | CA  | THR | 1096 | 99.185  | 50.411 | 21.762 | 1.00 | 30.51 |
| ATOM | 3901 | CB  | THR | 1096 | 100.229 | 50.384 | 20.647 | 1.00 | 31.43 |
| ATOM | 3902 | OG1 | THR | 1096 | 100.530 | 51.722 | 20.243 | 1.00 | 34.77 |
| ATOM | 3903 | CG2 | THR | 1096 | 99.706  | 49.629 | 19.445 | 1.00 | 34.07 |
| ATOM | 3904 | C   | THR | 1096 | 99.659  | 51.379 | 22.835 | 1.00 | 28.94 |
| ATOM | 3905 | O   | THR | 1096 | 99.314  | 52.558 | 22.793 | 1.00 | 30.80 |
| ATOM | 3906 | N   | PRO | 1097 | 100.461 | 50.902 | 23.807 | 1.00 | 28.40 |
| ATOM | 3907 | CD  | PRO | 1097 | 100.925 | 49.519 | 24.021 | 1.00 | 28.11 |
| ATOM | 3908 | CA  | PRO | 1097 | 100.958 | 51.781 | 24.869 | 1.00 | 27.84 |
| ATOM | 3909 | CB  | PRO | 1097 | 101.916 | 50.878 | 25.632 | 1.00 | 26.37 |
| ATOM | 3910 | CG  | PRO | 1097 | 101.293 | 49.531 | 25.481 | 1.00 | 25.06 |
| ATOM | 3911 | C   | PRO | 1097 | 101.689 | 52.956 | 24.258 | 1.00 | 29.88 |
| ATOM | 3912 | O   | PRO | 1097 | 101.583 | 54.084 | 24.739 | 1.00 | 30.91 |
| ATOM | 3913 | N   | GLU | 1098 | 102.384 | 52.683 | 23.156 | 1.00 | 32.60 |
| ATOM | 3914 | CA  | GLU | 1098 | 103.153 | 53.686 | 22.420 | 1.00 | 35.02 |
| ATOM | 3915 | CB  | GLU | 1098 | 103.974 | 53.017 | 21.310 | 1.00 | 37.79 |
| ATOM | 3916 | CG  | GLU | 1098 | 105.119 | 52.122 | 21.796 | 1.00 | 44.17 |
| ATOM | 3917 | CD  | GLU | 1098 | 104.669 | 50.740 | 22.271 | 1.00 | 48.86 |
| ATOM | 3918 | OE1 | GLU | 1098 | 103.779 | 50.132 | 21.628 | 1.00 | 49.58 |
| ATOM | 3919 | OE2 | GLU | 1098 | 105.229 | 50.256 | 23.281 | 1.00 | 49.09 |
| ATOM | 3920 | C   | GLU | 1098 | 102.269 | 54.787 | 21.814 | 1.00 | 35.22 |
| ATOM | 3921 | O   | GLU | 1098 | 102.590 | 55.975 | 21.907 | 1.00 | 35.11 |
| ATOM | 3922 | N   | PHE | 1099 | 101.170 | 54.378 | 21.182 | 1.00 | 34.71 |
| ATOM | 3923 | CA  | PHE | 1099 | 100.217 | 55.295 | 20.550 | 1.00 | 31.99 |
| ATOM | 3924 | CB  | PHE | 1099 | 99.114  | 54.487 | 19.854 | 1.00 | 30.86 |
| ATOM | 3925 | CG  | PHE | 1099 | 97.961  | 55.316 | 19.356 | 1.00 | 30.84 |
| ATOM | 3926 | CD1 | PHE | 1099 | 97.896  | 55.708 | 18.027 | 1.00 | 30.84 |
| ATOM | 3927 | CD2 | PHE | 1099 | 96.906  | 55.654 | 20.203 | 1.00 | 30.22 |
| ATOM | 3928 | CE1 | PHE | 1099 | 96.795  | 56.418 | 17.543 | 1.00 | 32.30 |
| ATOM | 3929 | CE2 | PHE | 1099 | 95.807  | 56.360 | 19.730 | 1.00 | 29.93 |
| ATOM | 3930 | CZ  | PHE | 1099 | 95.750  | 56.742 | 18.395 | 1.00 | 30.84 |
| ATOM | 3931 | C   | PHE | 1099 | 99.591  | 56.202 | 21.591 | 1.00 | 30.63 |
| ATOM | 3932 | O   | PHE | 1099 | 99.468  | 57.412 | 21.385 | 1.00 | 29.46 |
| ATOM | 3933 | N   | GLN | 1100 | 99.169  | 55.592 | 22.694 | 1.00 | 31.39 |
| ATOM | 3934 | CA  | GLN | 1100 | 98.535  | 56.312 | 23.782 | 1.00 | 33.54 |
| ATOM | 3935 | CB  | GLN | 1100 | 98.087  | 55.341 | 24.873 | 1.00 | 33.46 |
| ATOM | 3936 | CG  | GLN | 1100 | 97.206  | 56.000 | 25.918 | 1.00 | 33.43 |
| ATOM | 3937 | CD  | GLN | 1100 | 96.860  | 55.082 | 27.061 | 1.00 | 31.11 |
| ATOM | 3938 | OE1 | GLN | 1100 | 97.552  | 54.111 | 27.321 | 1.00 | 30.24 |
| ATOM | 3939 | NE2 | GLN | 1100 | 95.784  | 55.397 | 27.765 | 1.00 | 34.07 |
| ATOM | 3940 | C   | GLN | 1100 | 99.497  | 57.342 | 24.354 | 1.00 | 35.00 |
| ATOM | 3941 | O   | GLN | 1100 | 99.145  | 58.518 | 24.499 | 1.00 | 35.07 |

FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 3942 | N   | ALA | 1101 | 100.714 | 56.895 | 24.665 | 1.00 | 35.47 |
| ATOM | 3943 | CA  | ALA | 1101 | 101.752 | 57.772 | 25.206 | 1.00 | 34.10 |
| ATOM | 3944 | CB  | ALA | 1101 | 103.010 | 56.973 | 25.524 | 1.00 | 34.60 |
| ATOM | 3945 | C   | ALA | 1101 | 102.062 | 58.868 | 24.192 | 1.00 | 33.13 |
| ATOM | 3946 | O   | ALA | 1101 | 102.335 | 60.008 | 24.564 | 1.00 | 33.43 |
| ATOM | 3947 | N   | ASN | 1102 | 102.004 | 58.515 | 22.911 | 1.00 | 31.74 |
| ATOM | 3948 | CA  | ASN | 1102 | 102.251 | 59.464 | 21.831 | 1.00 | 31.93 |
| ATOM | 3949 | CB  | ASN | 1102 | 102.220 | 58.754 | 20.478 | 1.00 | 35.75 |
| ATOM | 3950 | CG  | ASN | 1102 | 102.222 | 59.722 | 19.314 | 1.00 | 38.97 |
| ATOM | 3951 | OD1 | ASN | 1102 | 103.115 | 60.562 | 19.188 | 1.00 | 35.68 |
| ATOM | 3952 | ND2 | ASN | 1102 | 101.207 | 59.617 | 18.460 | 1.00 | 44.14 |
| ATOM | 3953 | C   | ASN | 1102 | 101.174 | 60.535 | 21.878 | 1.00 | 30.58 |
| ATOM | 3954 | O   | ASN | 1102 | 101.465 | 61.734 | 21.820 | 1.00 | 28.72 |
| ATOM | 3955 | N   | GLU | 1103 | 99.926  | 60.092 | 21.994 | 1.00 | 30.88 |
| ATOM | 3956 | CA  | GLU | 1103 | 98.797  | 61.008 | 22.081 | 1.00 | 31.29 |
| ATOM | 3957 | CB  | GLU | 1103 | 97.496  | 60.236 | 22.305 | 1.00 | 29.94 |
| ATOM | 3958 | CG  | GLU | 1103 | 97.107  | 59.345 | 21.143 | 1.00 | 26.07 |
| ATOM | 3959 | CD  | GLU | 1103 | 97.147  | 60.077 | 19.817 | 1.00 | 26.39 |
| ATOM | 3960 | OE1 | GLU | 1103 | 96.367  | 61.041 | 19.642 | 1.00 | 23.03 |
| ATOM | 3961 | OE2 | GLU | 1103 | 97.972  | 59.695 | 18.957 | 1.00 | 27.36 |
| ATOM | 3962 | C   | GLU | 1103 | 99.033  | 61.971 | 23.236 | 1.00 | 31.53 |
| ATOM | 3963 | O   | GLU | 1103 | 98.880  | 63.183 | 23.077 | 1.00 | 32.08 |
| ATOM | 3964 | N   | VAL | 1104 | 99.448  | 61.421 | 24.378 | 1.00 | 32.16 |
| ATOM | 3965 | CA  | VAL | 1104 | 99.731  | 62.201 | 25.585 | 1.00 | 33.27 |
| ATOM | 3966 | CB  | VAL | 1104 | 100.191 | 61.286 | 26.744 | 1.00 | 30.58 |
| ATOM | 3967 | CG1 | VAL | 1104 | 100.569 | 62.110 | 27.962 | 1.00 | 28.79 |
| ATOM | 3968 | CG2 | VAL | 1104 | 99.093  | 60.304 | 27.096 | 1.00 | 32.06 |
| ATOM | 3969 | C   | VAL | 1104 | 100.823 | 63.225 | 25.306 | 1.00 | 34.57 |
| ATOM | 3970 | O   | VAL | 1104 | 100.695 | 64.404 | 25.649 | 1.00 | 34.06 |
| ATOM | 3971 | N   | ARG | 1105 | 101.876 | 62.762 | 24.642 | 1.00 | 36.12 |
| ATOM | 3972 | CA  | ARG | 1105 | 103.020 | 63.591 | 24.291 | 1.00 | 37.17 |
| ATOM | 3973 | CB  | ARG | 1105 | 103.981 | 62.780 | 23.422 | 1.00 | 41.18 |
| ATOM | 3974 | CG  | ARG | 1105 | 105.100 | 63.589 | 22.822 | 1.00 | 48.61 |
| ATOM | 3975 | CD  | ARG | 1105 | 105.767 | 62.842 | 21.689 | 1.00 | 54.64 |
| ATOM | 3976 | NE  | ARG | 1105 | 106.570 | 63.746 | 20.872 | 1.00 | 59.97 |
| ATOM | 3977 | CZ  | ARG | 1105 | 106.096 | 64.448 | 19.845 | 1.00 | 63.88 |
| ATOM | 3978 | NH1 | ARG | 1105 | 104.816 | 64.349 | 19.494 | 1.00 | 63.25 |
| ATOM | 3979 | NH2 | ARG | 1105 | 106.899 | 65.269 | 19.180 | 1.00 | 67.43 |
| ATOM | 3980 | C   | ARG | 1105 | 102.572 | 64.848 | 23.552 | 1.00 | 35.76 |
| ATOM | 3981 | O   | ARG | 1105 | 102.880 | 65.968 | 23.966 | 1.00 | 34.77 |
| ATOM | 3982 | N   | LYS | 1106 | 101.805 | 64.649 | 22.485 | 1.00 | 34.78 |
| ATOM | 3983 | CA  | LYS | 1106 | 101.301 | 65.747 | 21.669 | 1.00 | 34.00 |
| ATOM | 3984 | CB  | LYS | 1106 | 100.467 | 65.198 | 20.514 | 1.00 | 32.67 |
| ATOM | 3985 | CG  | LYS | 1106 | 101.212 | 64.189 | 19.670 | 1.00 | 31.83 |
| ATOM | 3986 | CD  | LYS | 1106 | 100.416 | 63.780 | 18.457 | 1.00 | 34.20 |
| ATOM | 3987 | CE  | LYS | 1106 | 99.090  | 63.176 | 18.846 | 1.00 | 39.46 |
| ATOM | 3988 | NZ  | LYS | 1106 | 98.374  | 62.649 | 17.655 | 1.00 | 43.75 |
| ATOM | 3989 | C   | LYS | 1106 | 100.485 | 66.760 | 22.465 | 1.00 | 34.26 |
| ATOM | 3990 | O   | LYS | 1106 | 100.459 | 67.946 | 22.128 | 1.00 | 35.05 |
| ATOM | 3991 | N   | VAL | 1107 | 99.808  | 66.293 | 23.510 | 1.00 | 33.42 |
| ATOM | 3992 | CA  | VAL | 1107 | 99.002  | 67.178 | 24.338 | 1.00 | 33.04 |
| ATOM | 3993 | CB  | VAL | 1107 | 97.977  | 66.394 | 25.195 | 1.00 | 29.85 |
| ATOM | 3994 | CG1 | VAL | 1107 | 97.189  | 67.340 | 26.089 | 1.00 | 24.12 |
| ATOM | 3995 | CG2 | VAL | 1107 | 97.031  | 65.624 | 24.302 | 1.00 | 30.73 |
| ATOM | 3996 | C   | VAL | 1107 | 99.920  | 67.967 | 25.258 | 1.00 | 35.29 |
| ATOM | 3997 | O   | VAL | 1107 | 99.868  | 69.196 | 25.300 | 1.00 | 36.49 |
| ATOM | 3998 | N   | LYS | 1108 | 100.793 | 67.258 | 25.959 | 1.00 | 36.76 |
| ATOM | 3999 | CA  | LYS | 1108 | 101.710 | 67.892 | 26.888 | 1.00 | 38.65 |



FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 4116 | CA  | LYS | 1242 | 102.525 | 75.863 | 31.635 | 1.00 | 40.98 |
| ATOM | 4117 | CB  | LYS | 1242 | 103.130 | 77.162 | 31.102 | 1.00 | 46.48 |
| ATOM | 4118 | CG  | LYS | 1242 | 103.655 | 78.106 | 32.184 | 1.00 | 54.66 |
| ATOM | 4119 | CD  | LYS | 1242 | 104.504 | 79.227 | 31.567 | 1.00 | 63.33 |
| ATOM | 4120 | CE  | LYS | 1242 | 105.116 | 80.153 | 32.623 | 1.00 | 68.01 |
| ATOM | 4121 | NZ  | LYS | 1242 | 106.121 | 79.459 | 33.488 | 1.00 | 71.11 |
| ATOM | 4122 | C   | LYS | 1242 | 102.068 | 74.977 | 30.471 | 1.00 | 40.38 |
| ATOM | 4123 | O   | LYS | 1242 | 101.545 | 75.471 | 29.472 | 1.00 | 40.63 |
| ATOM | 4124 | N   | GLN | 1243 | 102.281 | 73.672 | 30.582 | 1.00 | 38.45 |
| ATOM | 4125 | CA  | GLN | 1243 | 101.863 | 72.749 | 29.531 | 1.00 | 37.94 |
| ATOM | 4126 | CB  | GLN | 1243 | 102.905 | 71.640 | 29.338 | 1.00 | 42.14 |
| ATOM | 4127 | CG  | GLN | 1243 | 104.293 | 72.126 | 28.894 | 1.00 | 50.87 |
| ATOM | 4128 | CD  | GLN | 1243 | 104.296 | 72.805 | 27.516 | 1.00 | 58.97 |
| ATOM | 4129 | OE1 | GLN | 1243 | 104.790 | 72.248 | 26.533 | 1.00 | 61.73 |
| ATOM | 4130 | NE2 | GLN | 1243 | 103.777 | 74.026 | 27.454 | 1.00 | 61.92 |
| ATOM | 4131 | C   | GLN | 1243 | 100.502 | 72.162 | 29.907 | 1.00 | 35.65 |
| ATOM | 4132 | O   | GLN | 1243 | 100.286 | 71.781 | 31.059 | 1.00 | 34.91 |
| ATOM | 4133 | N   | LEU | 1244 | 99.577  | 72.130 | 28.949 | 1.00 | 33.29 |
| ATOM | 4134 | CA  | LEU | 1244 | 98.221  | 71.614 | 29.176 | 1.00 | 29.46 |
| ATOM | 4135 | CB  | LEU | 1244 | 97.495  | 71.389 | 27.848 | 1.00 | 27.97 |
| ATOM | 4136 | CG  | LEU | 1244 | 97.232  | 72.570 | 26.922 | 1.00 | 25.53 |
| ATOM | 4137 | CD1 | LEU | 1244 | 96.497  | 72.069 | 25.701 | 1.00 | 23.64 |
| ATOM | 4138 | CD2 | LEU | 1244 | 96.426  | 73.639 | 27.631 | 1.00 | 26.68 |
| ATOM | 4139 | C   | LEU | 1244 | 98.174  | 70.315 | 29.964 | 1.00 | 26.37 |
| ATOM | 4140 | O   | LEU | 1244 | 98.990  | 69.423 | 29.759 | 1.00 | 25.40 |
| ATOM | 4141 | N   | LEU | 1245 | 97.203  | 70.208 | 30.861 | 1.00 | 24.19 |
| ATOM | 4142 | CA  | LEU | 1245 | 97.043  | 69.000 | 31.654 | 1.00 | 21.24 |
| ATOM | 4143 | CB  | LEU | 1245 | 96.010  | 69.226 | 32.750 | 1.00 | 17.87 |
| ATOM | 4144 | CG  | LEU | 1245 | 96.388  | 70.166 | 33.886 | 1.00 | 13.30 |
| ATOM | 4145 | CD1 | LEU | 1245 | 95.278  | 70.190 | 34.957 | 1.00 | 8.28  |
| ATOM | 4146 | CD2 | LEU | 1245 | 97.692  | 69.691 | 34.476 | 1.00 | 12.89 |
| ATOM | 4147 | C   | LEU | 1245 | 96.577  | 67.851 | 30.760 | 1.00 | 22.73 |
| ATOM | 4148 | O   | LEU | 1245 | 95.875  | 68.067 | 29.772 | 1.00 | 22.07 |
| ATOM | 4149 | N   | CYS | 1246 | 96.970  | 66.631 | 31.097 | 1.00 | 23.09 |
| ATOM | 4150 | CA  | CYS | 1246 | 96.561  | 65.481 | 30.311 | 1.00 | 24.22 |
| ATOM | 4151 | CB  | CYS | 1246 | 97.564  | 65.167 | 29.213 | 1.00 | 23.07 |
| ATOM | 4152 | SG  | CYS | 1246 | 96.980  | 63.858 | 28.114 | 1.00 | 28.22 |
| ATOM | 4153 | C   | CYS | 1246 | 96.409  | 64.271 | 31.199 | 1.00 | 25.46 |
| ATOM | 4154 | O   | CYS | 1246 | 97.177  | 64.087 | 32.149 | 1.00 | 26.61 |
| ATOM | 4155 | N   | GLY | 1247 | 95.405  | 63.457 | 30.899 | 1.00 | 24.77 |
| ATOM | 4156 | CA  | GLY | 1247 | 95.159  | 62.257 | 31.669 | 1.00 | 23.54 |
| ATOM | 4157 | C   | GLY | 1247 | 95.056  | 61.081 | 30.724 | 1.00 | 22.83 |
| ATOM | 4158 | O   | GLY | 1247 | 94.823  | 61.260 | 29.525 | 1.00 | 22.59 |
| ATOM | 4159 | N   | ALA | 1248 | 95.230  | 59.878 | 31.252 | 1.00 | 20.75 |
| ATOM | 4160 | CA  | ALA | 1248 | 95.150  | 58.678 | 30.437 | 1.00 | 20.33 |
| ATOM | 4161 | CB  | ALA | 1248 | 96.536  | 58.256 | 29.990 | 1.00 | 21.90 |
| ATOM | 4162 | C   | ALA | 1248 | 94.485  | 57.561 | 31.222 | 1.00 | 20.51 |
| ATOM | 4163 | O   | ALA | 1248 | 94.619  | 57.473 | 32.447 | 1.00 | 18.34 |
| ATOM | 4164 | N   | ALA | 1249 | 93.740  | 56.727 | 30.514 | 1.00 | 20.76 |
| ATOM | 4165 | CA  | ALA | 1249 | 93.050  | 55.622 | 31.140 | 1.00 | 22.52 |
| ATOM | 4166 | CB  | ALA | 1249 | 91.670  | 55.477 | 30.543 | 1.00 | 22.47 |
| ATOM | 4167 | C   | ALA | 1249 | 93.825  | 54.342 | 30.928 | 1.00 | 24.15 |
| ATOM | 4168 | O   | ALA | 1249 | 94.183  | 54.019 | 29.790 | 1.00 | 25.00 |
| ATOM | 4169 | N   | ILE | 1250 | 94.105  | 53.616 | 32.005 | 1.00 | 23.49 |
| ATOM | 4170 | CA  | ILE | 1250 | 94.794  | 52.341 | 31.860 | 1.00 | 24.48 |
| ATOM | 4171 | CB  | ILE | 1250 | 96.254  | 52.330 | 32.417 | 1.00 | 22.98 |
| ATOM | 4172 | CG2 | ILE | 1250 | 97.088  | 53.412 | 31.760 | 1.00 | 24.80 |
| ATOM | 4173 | CG1 | ILE | 1250 | 96.276  | 52.433 | 33.939 | 1.00 | 20.21 |

FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 4232 | N   | TYR | 1258 | 103.911 | 48.678 | 32.100 | 1.00 | 36.40 |
| ATOM | 4233 | CA  | TYR | 1258 | 104.809 | 49.189 | 31.164 | 1.00 | 36.55 |
| ATOM | 4234 | CB  | TYR | 1258 | 105.067 | 48.121 | 30.108 | 1.00 | 36.16 |
| ATOM | 4235 | CG  | TYR | 1258 | 105.807 | 48.636 | 28.901 | 1.00 | 37.86 |
| ATOM | 4236 | CD1 | TYR | 1258 | 107.115 | 49.115 | 29.004 | 1.00 | 37.73 |
| ATOM | 4237 | CE1 | TYR | 1258 | 107.794 | 49.573 | 27.883 | 1.00 | 39.68 |
| ATOM | 4238 | CD2 | TYR | 1258 | 105.203 | 48.630 | 27.648 | 1.00 | 41.35 |
| ATOM | 4239 | CE2 | TYR | 1258 | 105.872 | 49.084 | 26.525 | 1.00 | 42.25 |
| ATOM | 4240 | CZ  | TYR | 1258 | 107.162 | 49.548 | 26.644 | 1.00 | 42.30 |
| ATOM | 4241 | OH  | TYR | 1258 | 107.808 | 49.978 | 25.510 | 1.00 | 46.56 |
| ATOM | 4242 | C   | TYR | 1258 | 104.149 | 50.402 | 30.525 | 1.00 | 37.00 |
| ATOM | 4243 | O   | TYR | 1258 | 104.794 | 51.427 | 30.276 | 1.00 | 39.78 |
| ATOM | 4244 | N   | ARG | 1259 | 102.858 | 50.250 | 30.243 | 1.00 | 35.45 |
| ATOM | 4245 | CA  | ARG | 1259 | 102.029 | 51.299 | 29.665 | 1.00 | 33.10 |
| ATOM | 4246 | CB  | ARG | 1259 | 100.571 | 50.829 | 29.669 | 1.00 | 35.78 |
| ATOM | 4247 | CG  | ARG | 1259 | 99.531  | 51.895 | 29.376 | 1.00 | 37.91 |
| ATOM | 4248 | CD  | ARG | 1259 | 99.265  | 52.018 | 27.901 | 1.00 | 35.20 |
| ATOM | 4249 | NE  | ARG | 1259 | 98.672  | 50.807 | 27.350 | 1.00 | 32.06 |
| ATOM | 4250 | CZ  | ARG | 1259 | 97.749  | 50.790 | 26.396 | 1.00 | 26.80 |
| ATOM | 4251 | NH1 | ARG | 1259 | 97.295  | 51.923 | 25.883 | 1.00 | 25.25 |
| ATOM | 4252 | NH2 | ARG | 1259 | 97.331  | 49.634 | 25.907 | 1.00 | 23.32 |
| ATOM | 4253 | C   | ARG | 1259 | 102.169 | 52.521 | 30.558 | 1.00 | 30.96 |
| ATOM | 4254 | O   | ARG | 1259 | 102.497 | 53.609 | 30.098 | 1.00 | 31.64 |
| ATOM | 4255 | N   | LEU | 1260 | 101.983 | 52.309 | 31.853 | 1.00 | 30.09 |
| ATOM | 4256 | CA  | LEU | 1260 | 102.087 | 53.382 | 32.820 | 1.00 | 30.15 |
| ATOM | 4257 | CB  | LEU | 1260 | 101.862 | 52.848 | 34.237 | 1.00 | 26.22 |
| ATOM | 4258 | CG  | LEU | 1260 | 101.775 | 53.919 | 35.324 | 1.00 | 28.20 |
| ATOM | 4259 | CD1 | LEU | 1260 | 100.640 | 54.876 | 34.984 | 1.00 | 28.15 |
| ATOM | 4260 | CD2 | LEU | 1260 | 101.578 | 53.289 | 36.698 | 1.00 | 23.65 |
| ATOM | 4261 | C   | LEU | 1260 | 103.453 | 54.058 | 32.704 | 1.00 | 31.69 |
| ATOM | 4262 | O   | LEU | 1260 | 103.545 | 55.285 | 32.784 | 1.00 | 31.52 |
| ATOM | 4263 | N   | ASP | 1261 | 104.503 | 53.267 | 32.481 | 1.00 | 32.30 |
| ATOM | 4264 | CA  | ASP | 1261 | 105.855 | 53.811 | 32.347 | 1.00 | 32.19 |
| ATOM | 4265 | CB  | ASP | 1261 | 106.879 | 52.703 | 32.075 | 1.00 | 35.55 |
| ATOM | 4266 | CG  | ASP | 1261 | 107.187 | 51.867 | 33.304 | 1.00 | 40.79 |
| ATOM | 4267 | OD1 | ASP | 1261 | 107.086 | 52.388 | 34.434 | 1.00 | 40.34 |
| ATOM | 4268 | OD2 | ASP | 1261 | 107.547 | 50.680 | 33.136 | 1.00 | 45.81 |
| ATOM | 4269 | C   | ASP | 1261 | 105.918 | 54.821 | 31.212 | 1.00 | 31.49 |
| ATOM | 4270 | O   | ASP | 1261 | 106.286 | 55.983 | 31.421 | 1.00 | 30.59 |
| ATOM | 4271 | N   | LEU | 1262 | 105.520 | 54.377 | 30.021 | 1.00 | 28.76 |
| ATOM | 4272 | CA  | LEU | 1262 | 105.536 | 55.225 | 28.836 | 1.00 | 27.39 |
| ATOM | 4273 | CB  | LEU | 1262 | 105.089 | 54.431 | 27.606 | 1.00 | 25.44 |
| ATOM | 4274 | CG  | LEU | 1262 | 105.782 | 53.082 | 27.388 | 1.00 | 20.68 |
| ATOM | 4275 | CD1 | LEU | 1262 | 105.355 | 52.486 | 26.063 | 1.00 | 16.25 |
| ATOM | 4276 | CD2 | LEU | 1262 | 107.284 | 53.263 | 27.435 | 1.00 | 19.30 |
| ATOM | 4277 | C   | LEU | 1262 | 104.683 | 56.484 | 29.010 | 1.00 | 27.65 |
| ATOM | 4278 | O   | LEU | 1262 | 105.096 | 57.578 | 28.616 | 1.00 | 28.28 |
| ATOM | 4279 | N   | LEU | 1263 | 103.502 | 56.336 | 29.603 | 1.00 | 26.91 |
| ATOM | 4280 | CA  | LEU | 1263 | 102.615 | 57.476 | 29.837 | 1.00 | 25.75 |
| ATOM | 4281 | CB  | LEU | 1263 | 101.267 | 57.021 | 30.393 | 1.00 | 24.46 |
| ATOM | 4282 | CG  | LEU | 1263 | 100.379 | 56.129 | 29.534 | 1.00 | 21.80 |
| ATOM | 4283 | CD1 | LEU | 1263 | 99.135  | 55.764 | 30.338 | 1.00 | 14.76 |
| ATOM | 4284 | CD2 | LEU | 1263 | 100.030 | 56.831 | 28.216 | 1.00 | 18.42 |
| ATOM | 4285 | C   | LEU | 1263 | 103.254 | 58.430 | 30.833 | 1.00 | 25.07 |
| ATOM | 4286 | O   | LEU | 1263 | 103.218 | 59.642 | 30.650 | 1.00 | 24.45 |
| ATOM | 4287 | N   | ALA | 1264 | 103.811 | 57.867 | 31.901 | 1.00 | 26.55 |
| ATOM | 4288 | CA  | ALA | 1264 | 104.469 | 58.643 | 32.945 | 1.00 | 27.92 |
| ATOM | 4289 | CB  | ALA | 1264 | 105.004 | 57.727 | 34.030 | 1.00 | 26.27 |



FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 4290 | C   | ALA | 1264 | 105.609 | 59.400 | 32.301 | 1.00 | 29.62 |
| ATOM | 4291 | O   | ALA | 1264 | 105.830 | 60.578 | 32.587 | 1.00 | 31.44 |
| ATOM | 4292 | N   | LEU | 1265 | 106.282 | 58.718 | 31.379 | 1.00 | 30.37 |
| ATOM | 4293 | CA  | LEU | 1265 | 107.419 | 59.262 | 30.646 | 1.00 | 29.10 |
| ATOM | 4294 | CB  | LEU | 1265 | 108.104 | 58.150 | 29.859 | 1.00 | 28.95 |
| ATOM | 4295 | CG  | LEU | 1265 | 109.498 | 58.414 | 29.306 | 1.00 | 31.50 |
| ATOM | 4296 | CD1 | LEU | 1265 | 110.532 | 58.266 | 30.422 | 1.00 | 30.76 |
| ATOM | 4297 | CD2 | LEU | 1265 | 109.784 | 57.415 | 28.187 | 1.00 | 33.34 |
| ATOM | 4298 | C   | LEU | 1265 | 106.980 | 60.354 | 29.683 | 1.00 | 28.32 |
| ATOM | 4299 | O   | LEU | 1265 | 107.746 | 61.272 | 29.399 | 1.00 | 30.26 |
| ATOM | 4300 | N   | ALA | 1266 | 105.766 | 60.221 | 29.151 | 1.00 | 27.20 |
| ATOM | 4301 | CA  | ALA | 1266 | 105.212 | 61.196 | 28.209 | 1.00 | 24.22 |
| ATOM | 4302 | CB  | ALA | 1266 | 104.134 | 60.554 | 27.352 | 1.00 | 23.15 |
| ATOM | 4303 | C   | ALA | 1266 | 104.659 | 62.432 | 28.919 | 1.00 | 22.49 |
| ATOM | 4304 | O   | ALA | 1266 | 104.268 | 63.399 | 28.267 | 1.00 | 21.03 |
| ATOM | 4305 | N   | GLY | 1267 | 104.611 | 62.387 | 30.249 | 1.00 | 21.17 |
| ATOM | 4306 | CA  | GLY | 1267 | 104.127 | 63.523 | 31.014 | 1.00 | 22.19 |
| ATOM | 4307 | C   | GLY | 1267 | 102.648 | 63.543 | 31.355 | 1.00 | 22.76 |
| ATOM | 4308 | O   | GLY | 1267 | 102.041 | 64.613 | 31.431 | 1.00 | 21.01 |
| ATOM | 4309 | N   | VAL | 1268 | 102.065 | 62.372 | 31.591 | 1.00 | 23.69 |
| ATOM | 4310 | CA  | VAL | 1268 | 100.653 | 62.307 | 31.941 | 1.00 | 23.87 |
| ATOM | 4311 | CB  | VAL | 1268 | 100.080 | 60.893 | 31.731 | 1.00 | 20.71 |
| ATOM | 4312 | CG1 | VAL | 1268 | 100.520 | 59.964 | 32.826 | 1.00 | 17.95 |
| ATOM | 4313 | CG2 | VAL | 1268 | 98.578  | 60.950 | 31.626 | 1.00 | 20.64 |
| ATOM | 4314 | C   | VAL | 1268 | 100.452 | 62.771 | 33.384 | 1.00 | 25.49 |
| ATOM | 4315 | O   | VAL | 1268 | 101.144 | 62.322 | 34.303 | 1.00 | 26.11 |
| ATOM | 4316 | N   | ASP | 1269 | 99.518  | 63.697 | 33.566 | 1.00 | 25.93 |
| ATOM | 4317 | CA  | ASP | 1269 | 99.222  | 64.259 | 34.879 | 1.00 | 26.16 |
| ATOM | 4318 | CB  | ASP | 1269 | 98.559  | 65.635 | 34.722 | 1.00 | 28.20 |
| ATOM | 4319 | CG  | ASP | 1269 | 99.417  | 66.619 | 33.933 | 1.00 | 31.21 |
| ATOM | 4320 | OD1 | ASP | 1269 | 99.365  | 66.591 | 32.686 | 1.00 | 31.29 |
| ATOM | 4321 | OD2 | ASP | 1269 | 100.138 | 67.425 | 34.558 | 1.00 | 33.35 |
| ATOM | 4322 | C   | ASP | 1269 | 98.347  | 63.358 | 35.750 | 1.00 | 25.89 |
| ATOM | 4323 | O   | ASP | 1269 | 98.545  | 63.282 | 36.961 | 1.00 | 28.47 |
| ATOM | 4324 | N   | VAL | 1270 | 97.355  | 62.709 | 35.145 | 1.00 | 24.11 |
| ATOM | 4325 | CA  | VAL | 1270 | 96.455  | 61.833 | 35.889 | 1.00 | 21.61 |
| ATOM | 4326 | CB  | VAL | 1270 | 95.073  | 62.465 | 36.165 | 1.00 | 21.00 |
| ATOM | 4327 | CG1 | VAL | 1270 | 94.877  | 62.637 | 37.649 | 1.00 | 23.22 |
| ATOM | 4328 | CG2 | VAL | 1270 | 94.880  | 63.776 | 35.396 | 1.00 | 19.40 |
| ATOM | 4329 | C   | VAL | 1270 | 96.165  | 60.554 | 35.148 | 1.00 | 21.02 |
| ATOM | 4330 | O   | VAL | 1270 | 95.971  | 60.559 | 33.932 | 1.00 | 19.61 |
| ATOM | 4331 | N   | VAL | 1271 | 96.102  | 59.460 | 35.889 | 1.00 | 20.75 |
| ATOM | 4332 | CA  | VAL | 1271 | 95.790  | 58.183 | 35.290 | 1.00 | 22.08 |
| ATOM | 4333 | CB  | VAL | 1271 | 96.978  | 57.212 | 35.333 | 1.00 | 24.24 |
| ATOM | 4334 | CG1 | VAL | 1271 | 96.520  | 55.814 | 34.937 | 1.00 | 20.83 |
| ATOM | 4335 | CG2 | VAL | 1271 | 98.078  | 57.697 | 34.380 | 1.00 | 25.92 |
| ATOM | 4336 | C   | VAL | 1271 | 94.590  | 57.598 | 36.014 | 1.00 | 23.47 |
| ATOM | 4337 | O   | VAL | 1271 | 94.499  | 57.643 | 37.246 | 1.00 | 22.00 |
| ATOM | 4338 | N   | VAL | 1272 | 93.641  | 57.111 | 35.227 | 1.00 | 23.18 |
| ATOM | 4339 | CA  | VAL | 1272 | 92.437  | 56.526 | 35.761 | 1.00 | 21.99 |
| ATOM | 4340 | CB  | VAL | 1272 | 91.168  | 57.241 | 35.221 | 1.00 | 25.19 |
| ATOM | 4341 | CG1 | VAL | 1272 | 91.239  | 57.393 | 33.715 | 1.00 | 25.64 |
| ATOM | 4342 | CG2 | VAL | 1272 | 89.900  | 56.475 | 35.637 | 1.00 | 26.87 |
| ATOM | 4343 | C   | VAL | 1272 | 92.393  | 55.052 | 35.421 | 1.00 | 22.23 |
| ATOM | 4344 | O   | VAL | 1272 | 92.586  | 54.654 | 34.266 | 1.00 | 21.79 |
| ATOM | 4345 | N   | LEU | 1273 | 92.195  | 54.241 | 36.448 | 1.00 | 21.58 |
| ATOM | 4346 | CA  | LEU | 1273 | 92.103  | 52.812 | 36.265 | 1.00 | 21.13 |
| ATOM | 4347 | CB  | LEU | 1273 | 92.339  | 52.122 | 37.605 | 1.00 | 24.63 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 4406 | C   | ILE | 1281 | 92.901 | 43.473 | 43.486 | 1.00 | 17.34 |
| ATOM | 4407 | O   | ILE | 1281 | 93.942 | 44.057 | 43.733 | 1.00 | 17.63 |
| ATOM | 4408 | N   | PHE | 1282 | 92.540 | 43.128 | 42.255 | 1.00 | 18.73 |
| ATOM | 4409 | CA  | PHE | 1282 | 93.385 | 43.402 | 41.092 | 1.00 | 20.07 |
| ATOM | 4410 | CB  | PHE | 1282 | 92.670 | 43.005 | 39.795 | 1.00 | 17.08 |
| ATOM | 4411 | CG  | PHE | 1282 | 92.159 | 41.588 | 39.792 | 1.00 | 22.43 |
| ATOM | 4412 | CD1 | PHE | 1282 | 93.039 | 40.515 | 39.820 | 1.00 | 26.46 |
| ATOM | 4413 | CD2 | PHE | 1282 | 90.794 | 41.325 | 39.785 | 1.00 | 26.55 |
| ATOM | 4414 | CE1 | PHE | 1282 | 92.563 | 39.201 | 39.843 | 1.00 | 30.07 |
| ATOM | 4415 | CE2 | PHE | 1282 | 90.309 | 40.014 | 39.808 | 1.00 | 25.06 |
| ATOM | 4416 | CZ  | PHE | 1282 | 91.192 | 38.956 | 39.838 | 1.00 | 27.50 |
| ATOM | 4417 | C   | PHE | 1282 | 93.705 | 44.888 | 41.066 | 1.00 | 22.54 |
| ATOM | 4418 | O   | PHE | 1282 | 94.874 | 45.287 | 41.056 | 1.00 | 25.62 |
| ATOM | 4419 | N   | GLN | 1283 | 92.661 | 45.709 | 41.115 | 1.00 | 22.95 |
| ATOM | 4420 | CA  | GLN | 1283 | 92.832 | 47.146 | 41.093 | 1.00 | 21.25 |
| ATOM | 4421 | CB  | GLN | 1283 | 91.511 | 47.840 | 40.854 | 1.00 | 22.07 |
| ATOM | 4422 | CG  | GLN | 1283 | 91.664 | 49.331 | 40.945 | 1.00 | 26.78 |
| ATOM | 4423 | CD  | GLN | 1283 | 90.504 | 50.068 | 40.363 | 1.00 | 25.14 |
| ATOM | 4424 | OE1 | GLN | 1283 | 90.003 | 51.012 | 40.961 | 1.00 | 25.91 |
| ATOM | 4425 | NE2 | GLN | 1283 | 90.077 | 49.658 | 39.178 | 1.00 | 27.92 |
| ATOM | 4426 | C   | GLN | 1283 | 93.462 | 47.689 | 42.360 | 1.00 | 21.70 |
| ATOM | 4427 | O   | GLN | 1283 | 94.318 | 48.564 | 42.290 | 1.00 | 22.53 |
| ATOM | 4428 | N   | ILE | 1284 | 93.002 | 47.207 | 43.512 | 1.00 | 22.32 |
| ATOM | 4429 | CA  | ILE | 1284 | 93.535 | 47.628 | 44.813 | 1.00 | 22.57 |
| ATOM | 4430 | CB  | ILE | 1284 | 92.981 | 46.745 | 45.976 | 1.00 | 22.24 |
| ATOM | 4431 | CG2 | ILE | 1284 | 93.803 | 46.933 | 47.237 | 1.00 | 24.28 |
| ATOM | 4432 | CG1 | ILE | 1284 | 91.519 | 47.079 | 46.267 | 1.00 | 19.88 |
| ATOM | 4433 | CD1 | ILE | 1284 | 90.888 | 46.144 | 47.282 | 1.00 | 18.19 |
| ATOM | 4434 | C   | ILE | 1284 | 95.053 | 47.490 | 44.800 | 1.00 | 23.74 |
| ATOM | 4435 | O   | ILE | 1284 | 95.775 | 48.376 | 45.271 | 1.00 | 26.46 |
| ATOM | 4436 | N   | ASN | 1285 | 95.532 | 46.372 | 44.267 | 1.00 | 22.44 |
| ATOM | 4437 | CA  | ASN | 1285 | 96.961 | 46.124 | 44.198 | 1.00 | 23.17 |
| ATOM | 4438 | CB  | ASN | 1285 | 97.253 | 44.684 | 43.759 | 1.00 | 20.77 |
| ATOM | 4439 | CG  | ASN | 1285 | 97.072 | 43.669 | 44.887 | 1.00 | 20.36 |
| ATOM | 4440 | OD1 | ASN | 1285 | 96.805 | 42.490 | 44.631 | 1.00 | 24.13 |
| ATOM | 4441 | ND2 | ASN | 1285 | 97.246 | 44.108 | 46.128 | 1.00 | 14.74 |
| ATOM | 4442 | C   | ASN | 1285 | 97.617 | 47.117 | 43.246 | 1.00 | 25.34 |
| ATOM | 4443 | O   | ASN | 1285 | 98.677 | 47.666 | 43.546 | 1.00 | 28.24 |
| ATOM | 4444 | N   | MET | 1286 | 96.963 | 47.387 | 42.124 | 1.00 | 25.91 |
| ATOM | 4445 | CA  | MET | 1286 | 97.505 | 48.323 | 41.152 | 1.00 | 28.16 |
| ATOM | 4446 | CB  | MET | 1286 | 96.630 | 48.363 | 39.902 | 1.00 | 28.67 |
| ATOM | 4447 | CG  | MET | 1286 | 97.171 | 49.264 | 38.799 | 1.00 | 36.28 |
| ATOM | 4448 | SD  | MET | 1286 | 98.715 | 48.689 | 38.035 | 1.00 | 38.55 |
| ATOM | 4449 | CE  | MET | 1286 | 98.426 | 49.121 | 36.310 | 1.00 | 33.76 |
| ATOM | 4450 | C   | MET | 1286 | 97.648 | 49.731 | 41.738 | 1.00 | 29.19 |
| ATOM | 4451 | O   | MET | 1286 | 98.662 | 50.393 | 41.527 | 1.00 | 30.56 |
| ATOM | 4452 | N   | ILE | 1287 | 96.652 | 50.174 | 42.501 | 1.00 | 27.85 |
| ATOM | 4453 | CA  | ILE | 1287 | 96.688 | 51.502 | 43.092 | 1.00 | 25.81 |
| ATOM | 4454 | CB  | ILE | 1287 | 95.405 | 51.813 | 43.873 | 1.00 | 24.59 |
| ATOM | 4455 | CG2 | ILE | 1287 | 95.458 | 53.237 | 44.415 | 1.00 | 25.47 |
| ATOM | 4456 | CG1 | ILE | 1287 | 94.193 | 51.660 | 42.953 | 1.00 | 22.46 |
| ATOM | 4457 | CD1 | ILE | 1287 | 92.874 | 51.620 | 43.673 | 1.00 | 23.78 |
| ATOM | 4458 | C   | ILE | 1287 | 97.891 | 51.643 | 44.005 | 1.00 | 26.84 |
| ATOM | 4459 | O   | ILE | 1287 | 98.594 | 52.654 | 43.950 | 1.00 | 28.07 |
| ATOM | 4460 | N   | LYS | 1288 | 98.143 | 50.623 | 44.820 | 1.00 | 27.20 |
| ATOM | 4461 | CA  | LYS | 1288 | 99.284 | 50.640 | 45.736 | 1.00 | 27.46 |
| ATOM | 4462 | CB  | LYS | 1288 | 99.252 | 49.417 | 46.650 | 1.00 | 30.05 |
| ATOM | 4463 | CG  | LYS | 1288 | 98.036 | 49.335 | 47.562 | 1.00 | 30.55 |

FIGURE 1 (CONT.)

|      |      |     |     |      |         |        |        |      |       |
|------|------|-----|-----|------|---------|--------|--------|------|-------|
| ATOM | 4464 | CD  | LYS | 1288 | 98.070  | 48.045 | 48.367 | 1.00 | 32.83 |
| ATOM | 4465 | CE  | LYS | 1288 | 96.838  | 47.890 | 49.229 | 1.00 | 39.32 |
| ATOM | 4466 | NZ  | LYS | 1288 | 96.699  | 49.020 | 50.186 | 1.00 | 47.11 |
| ATOM | 4467 | C   | LYS | 1288 | 100.596 | 50.673 | 44.951 | 1.00 | 27.26 |
| ATOM | 4468 | O   | LYS | 1288 | 101.502 | 51.438 | 45.273 | 1.00 | 27.28 |
| ATOM | 4469 | N   | TYR | 1289 | 100.684 | 49.846 | 43.914 | 1.00 | 27.29 |
| ATOM | 4470 | CA  | TYR | 1289 | 101.865 | 49.791 | 43.056 | 1.00 | 28.47 |
| ATOM | 4471 | CB  | TYR | 1289 | 101.625 | 48.799 | 41.903 | 1.00 | 28.60 |
| ATOM | 4472 | CG  | TYR | 1289 | 102.557 | 48.960 | 40.722 | 1.00 | 28.87 |
| ATOM | 4473 | CD1 | TYR | 1289 | 102.192 | 49.728 | 39.614 | 1.00 | 29.46 |
| ATOM | 4474 | CE1 | TYR | 1289 | 103.069 | 49.914 | 38.547 | 1.00 | 31.03 |
| ATOM | 4475 | CD2 | TYR | 1289 | 103.820 | 48.375 | 40.728 | 1.00 | 31.59 |
| ATOM | 4476 | CE2 | TYR | 1289 | 104.708 | 48.553 | 39.664 | 1.00 | 29.02 |
| ATOM | 4477 | CZ  | TYR | 1289 | 104.327 | 49.321 | 38.531 | 1.00 | 31.10 |
| ATOM | 4478 | OH  | TYR | 1289 | 105.207 | 49.484 | 37.536 | 1.00 | 30.82 |
| ATOM | 4479 | C   | TYR | 1289 | 102.193 | 51.180 | 42.493 | 1.00 | 28.78 |
| ATOM | 4480 | O   | TYR | 1289 | 103.305 | 51.669 | 42.641 | 1.00 | 29.48 |
| ATOM | 4481 | N   | MET | 1290 | 101.201 | 51.816 | 41.883 | 1.00 | 29.89 |
| ATOM | 4482 | CA  | MET | 1290 | 101.348 | 53.133 | 41.276 | 1.00 | 30.44 |
| ATOM | 4483 | CB  | MET | 1290 | 100.028 | 53.561 | 40.643 | 1.00 | 31.57 |
| ATOM | 4484 | CG  | MET | 1290 | 99.579  | 52.680 | 39.497 | 1.00 | 33.84 |
| ATOM | 4485 | SD  | MET | 1290 | 98.003  | 53.207 | 38.816 | 1.00 | 34.81 |
| ATOM | 4486 | CE  | MET | 1290 | 98.487  | 54.694 | 37.920 | 1.00 | 30.99 |
| ATOM | 4487 | C   | MET | 1290 | 101.822 | 54.226 | 42.225 | 1.00 | 32.79 |
| ATOM | 4488 | O   | MET | 1290 | 102.509 | 55.159 | 41.804 | 1.00 | 31.48 |
| ATOM | 4489 | N   | LYS | 1291 | 101.417 | 54.139 | 43.489 | 1.00 | 35.25 |
| ATOM | 4490 | CA  | LYS | 1291 | 101.810 | 55.132 | 44.487 | 1.00 | 37.17 |
| ATOM | 4491 | CB  | LYS | 1291 | 100.763 | 55.209 | 45.602 | 1.00 | 38.08 |
| ATOM | 4492 | CG  | LYS | 1291 | 99.336  | 55.394 | 45.099 | 1.00 | 36.81 |
| ATOM | 4493 | CD  | LYS | 1291 | 99.172  | 56.661 | 44.268 | 1.00 | 38.58 |
| ATOM | 4494 | CE  | LYS | 1291 | 99.288  | 57.907 | 45.130 | 1.00 | 38.10 |
| ATOM | 4495 | NZ  | LYS | 1291 | 99.087  | 59.155 | 44.349 | 1.00 | 34.25 |
| ATOM | 4496 | C   | LYS | 1291 | 103.196 | 54.824 | 45.053 | 1.00 | 38.96 |
| ATOM | 4497 | O   | LYS | 1291 | 103.878 | 55.711 | 45.563 | 1.00 | 39.01 |
| ATOM | 4498 | N   | GLU | 1292 | 103.592 | 53.556 | 44.994 | 1.00 | 41.96 |
| ATOM | 4499 | CA  | GLU | 1292 | 104.916 | 53.144 | 45.456 | 1.00 | 45.55 |
| ATOM | 4500 | CB  | GLU | 1292 | 105.037 | 51.608 | 45.509 | 1.00 | 51.52 |
| ATOM | 4501 | CG  | GLU | 1292 | 104.263 | 50.910 | 46.636 | 1.00 | 62.57 |
| ATOM | 4502 | CD  | GLU | 1292 | 104.341 | 49.374 | 46.570 | 1.00 | 68.88 |
| ATOM | 4503 | OE1 | GLU | 1292 | 103.372 | 48.706 | 47.005 | 1.00 | 67.53 |
| ATOM | 4504 | OE2 | GLU | 1292 | 105.366 | 48.833 | 46.090 | 1.00 | 72.18 |
| ATOM | 4505 | C   | GLU | 1292 | 105.907 | 53.672 | 44.417 | 1.00 | 44.62 |
| ATOM | 4506 | O   | GLU | 1292 | 106.841 | 54.406 | 44.740 | 1.00 | 46.70 |
| ATOM | 4507 | N   | LYS | 1293 | 105.642 | 53.333 | 43.159 | 1.00 | 42.18 |
| ATOM | 4508 | CA  | LYS | 1293 | 106.485 | 53.724 | 42.041 | 1.00 | 39.72 |
| ATOM | 4509 | CB  | LYS | 1293 | 106.106 | 52.921 | 40.799 | 1.00 | 36.18 |
| ATOM | 4510 | CG  | LYS | 1293 | 107.107 | 53.036 | 39.677 | 1.00 | 34.73 |
| ATOM | 4511 | CD  | LYS | 1293 | 106.759 | 52.096 | 38.554 | 1.00 | 34.72 |
| ATOM | 4512 | CE  | LYS | 1293 | 107.897 | 51.979 | 37.575 | 1.00 | 34.77 |
| ATOM | 4513 | NZ  | LYS | 1293 | 109.072 | 51.348 | 38.214 | 1.00 | 35.52 |
| ATOM | 4514 | C   | LYS | 1293 | 106.464 | 55.214 | 41.719 | 1.00 | 39.53 |
| ATOM | 4515 | O   | LYS | 1293 | 107.513 | 55.821 | 41.526 | 1.00 | 40.47 |
| ATOM | 4516 | N   | TYR | 1294 | 105.278 | 55.800 | 41.650 | 1.00 | 39.92 |
| ATOM | 4517 | CA  | TYR | 1294 | 105.139 | 57.217 | 41.333 | 1.00 | 41.35 |
| ATOM | 4518 | CB  | TYR | 1294 | 104.370 | 57.373 | 40.019 | 1.00 | 39.56 |
| ATOM | 4519 | CG  | TYR | 1294 | 105.002 | 56.664 | 38.846 | 1.00 | 37.42 |
| ATOM | 4520 | CD1 | TYR | 1294 | 106.057 | 57.248 | 38.146 | 1.00 | 34.52 |
| ATOM | 4521 | CE1 | TYR | 1294 | 106.647 | 56.609 | 37.074 | 1.00 | 30.70 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 4580 | CA  | GLY | 1302 | 87.841 | 51.757 | 38.899 | 1.00 | 27.86 |
| ATOM | 4581 | C   | GLY | 1302 | 86.635 | 52.519 | 38.468 | 1.00 | 29.36 |
| ATOM | 4582 | O   | GLY | 1302 | 86.703 | 53.334 | 37.558 | 1.00 | 34.73 |
| ATOM | 4583 | N   | ASN | 1303 | 85.521 | 52.201 | 39.105 | 1.00 | 26.96 |
| ATOM | 4584 | CA  | ASN | 1303 | 84.243 | 52.853 | 38.878 | 1.00 | 22.20 |
| ATOM | 4585 | CB  | ASN | 1303 | 83.665 | 52.538 | 37.502 | 1.00 | 19.58 |
| ATOM | 4586 | CG  | ASN | 1303 | 83.615 | 53.764 | 36.600 | 1.00 | 21.65 |
| ATOM | 4587 | OD1 | ASN | 1303 | 84.623 | 54.160 | 36.019 | 1.00 | 23.46 |
| ATOM | 4588 | ND2 | ASN | 1303 | 82.441 | 54.373 | 36.483 | 1.00 | 19.93 |
| ATOM | 4589 | C   | ASN | 1303 | 83.405 | 52.256 | 39.975 | 1.00 | 21.48 |
| ATOM | 4590 | O   | ASN | 1303 | 83.237 | 51.031 | 40.036 | 1.00 | 23.60 |
| ATOM | 4591 | N   | VAL | 1304 | 83.008 | 53.104 | 40.917 | 1.00 | 19.16 |
| ATOM | 4592 | CA  | VAL | 1304 | 82.219 | 52.680 | 42.064 | 1.00 | 15.46 |
| ATOM | 4593 | CB  | VAL | 1304 | 82.972 | 52.975 | 43.389 | 1.00 | 12.26 |
| ATOM | 4594 | CG1 | VAL | 1304 | 84.255 | 52.158 | 43.465 | 1.00 | 11.22 |
| ATOM | 4595 | CG2 | VAL | 1304 | 83.279 | 54.464 | 43.512 | 1.00 | 6.37  |
| ATOM | 4596 | C   | VAL | 1304 | 80.851 | 53.346 | 42.131 | 1.00 | 15.07 |
| ATOM | 4597 | O   | VAL | 1304 | 80.628 | 54.392 | 41.527 | 1.00 | 14.88 |
| ATOM | 4598 | N   | VAL | 1305 | 79.921 | 52.707 | 42.833 | 1.00 | 15.51 |
| ATOM | 4599 | CA  | VAL | 1305 | 78.583 | 53.256 | 43.023 | 1.00 | 16.66 |
| ATOM | 4600 | CB  | VAL | 1305 | 77.522 | 52.568 | 42.135 | 1.00 | 11.85 |
| ATOM | 4601 | CG1 | VAL | 1305 | 77.863 | 52.742 | 40.686 | 1.00 | 16.33 |
| ATOM | 4602 | CG2 | VAL | 1305 | 77.387 | 51.113 | 42.484 | 1.00 | 9.15  |
| ATOM | 4603 | C   | VAL | 1305 | 78.162 | 53.113 | 44.484 | 1.00 | 19.22 |
| ATOM | 4604 | O   | VAL | 1305 | 77.079 | 53.565 | 44.871 | 1.00 | 21.20 |
| ATOM | 4605 | N   | THR | 1306 | 79.049 | 52.550 | 45.302 | 1.00 | 19.23 |
| ATOM | 4606 | CA  | THR | 1306 | 78.757 | 52.328 | 46.715 | 1.00 | 19.71 |
| ATOM | 4607 | CB  | THR | 1306 | 78.495 | 50.838 | 46.959 | 1.00 | 18.95 |
| ATOM | 4608 | OG1 | THR | 1306 | 77.323 | 50.444 | 46.239 | 1.00 | 19.72 |
| ATOM | 4609 | CG2 | THR | 1306 | 78.309 | 50.546 | 48.425 | 1.00 | 23.97 |
| ATOM | 4610 | C   | THR | 1306 | 79.843 | 52.805 | 47.683 | 1.00 | 19.97 |
| ATOM | 4611 | O   | THR | 1306 | 81.036 | 52.772 | 47.374 | 1.00 | 19.43 |
| ATOM | 4612 | N   | ALA | 1307 | 79.411 | 53.232 | 48.866 | 1.00 | 20.52 |
| ATOM | 4613 | CA  | ALA | 1307 | 80.310 | 53.703 | 49.908 | 1.00 | 20.85 |
| ATOM | 4614 | CB  | ALA | 1307 | 79.502 | 54.112 | 51.123 | 1.00 | 20.42 |
| ATOM | 4615 | C   | ALA | 1307 | 81.341 | 52.624 | 50.282 | 1.00 | 22.03 |
| ATOM | 4616 | O   | ALA | 1307 | 82.516 | 52.922 | 50.508 | 1.00 | 23.72 |
| ATOM | 4617 | N   | ALA | 1308 | 80.897 | 51.372 | 50.323 | 1.00 | 20.40 |
| ATOM | 4618 | CA  | ALA | 1308 | 81.761 | 50.245 | 50.653 | 1.00 | 18.53 |
| ATOM | 4619 | CB  | ALA | 1308 | 80.937 | 48.987 | 50.770 | 1.00 | 21.04 |
| ATOM | 4620 | C   | ALA | 1308 | 82.870 | 50.059 | 49.623 | 1.00 | 18.54 |
| ATOM | 4621 | O   | ALA | 1308 | 84.023 | 49.828 | 49.983 | 1.00 | 22.02 |
| ATOM | 4622 | N   | GLN | 1309 | 82.517 | 50.135 | 48.344 | 1.00 | 16.74 |
| ATOM | 4623 | CA  | GLN | 1309 | 83.498 | 50.009 | 47.276 | 1.00 | 18.03 |
| ATOM | 4624 | CB  | GLN | 1309 | 82.828 | 50.091 | 45.913 | 1.00 | 20.48 |
| ATOM | 4625 | CG  | GLN | 1309 | 81.908 | 48.962 | 45.530 | 1.00 | 16.20 |
| ATOM | 4626 | CD  | GLN | 1309 | 81.190 | 49.286 | 44.240 | 1.00 | 16.50 |
| ATOM | 4627 | OE1 | GLN | 1309 | 80.346 | 50.187 | 44.202 | 1.00 | 18.85 |
| ATOM | 4628 | NE2 | GLN | 1309 | 81.552 | 48.599 | 43.164 | 1.00 | 12.20 |
| ATOM | 4629 | C   | GLN | 1309 | 84.468 | 51.179 | 47.376 | 1.00 | 19.43 |
| ATOM | 4630 | O   | GLN | 1309 | 85.679 | 51.011 | 47.245 | 1.00 | 21.03 |
| ATOM | 4631 | N   | ALA | 1310 | 83.916 | 52.373 | 47.569 | 1.00 | 20.11 |
| ATOM | 4632 | CA  | ALA | 1310 | 84.718 | 53.586 | 47.686 | 1.00 | 21.85 |
| ATOM | 4633 | CB  | ALA | 1310 | 83.817 | 54.794 | 47.940 | 1.00 | 20.77 |
| ATOM | 4634 | C   | ALA | 1310 | 85.771 | 53.463 | 48.791 | 1.00 | 22.24 |
| ATOM | 4635 | O   | ALA | 1310 | 86.928 | 53.834 | 48.593 | 1.00 | 22.99 |
| ATOM | 4636 | N   | LYS | 1311 | 85.384 | 52.886 | 49.924 | 1.00 | 21.35 |
| ATOM | 4637 | CA  | LYS | 1311 | 86.295 | 52.719 | 51.050 | 1.00 | 22.31 |

# FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 4696 | CG  | ASP | 1319 | 95.637 | 60.944 | 44.391 | 1.00 | 27.24 |
| ATOM | 4697 | OD1 | ASP | 1319 | 96.101 | 61.403 | 45.454 | 1.00 | 29.40 |
| ATOM | 4698 | OD2 | ASP | 1319 | 96.252 | 60.129 | 43.678 | 1.00 | 29.66 |
| ATOM | 4699 | C   | ASP | 1319 | 91.793 | 61.284 | 44.397 | 1.00 | 23.19 |
| ATOM | 4700 | O   | ASP | 1319 | 91.499 | 62.450 | 44.692 | 1.00 | 22.82 |
| ATOM | 4701 | N   | ALA | 1320 | 90.985 | 60.469 | 43.717 | 1.00 | 21.37 |
| ATOM | 4702 | CA  | ALA | 1320 | 89.648 | 60.837 | 43.248 | 1.00 | 18.83 |
| ATOM | 4703 | CB  | ALA | 1320 | 89.734 | 61.685 | 41.991 | 1.00 | 17.58 |
| ATOM | 4704 | C   | ALA | 1320 | 88.921 | 59.544 | 42.934 | 1.00 | 19.14 |
| ATOM | 4705 | O   | ALA | 1320 | 89.555 | 58.500 | 42.779 | 1.00 | 21.36 |
| ATOM | 4706 | N   | LEU | 1321 | 87.600 | 59.606 | 42.817 | 1.00 | 18.91 |
| ATOM | 4707 | CA  | LEU | 1321 | 86.806 | 58.417 | 42.512 | 1.00 | 18.35 |
| ATOM | 4708 | CB  | LEU | 1321 | 85.902 | 58.065 | 43.697 | 1.00 | 19.13 |
| ATOM | 4709 | CG  | LEU | 1321 | 86.535 | 57.340 | 44.889 | 1.00 | 18.32 |
| ATOM | 4710 | CD1 | LEU | 1321 | 85.605 | 57.384 | 46.085 | 1.00 | 18.96 |
| ATOM | 4711 | CD2 | LEU | 1321 | 86.850 | 55.905 | 44.510 | 1.00 | 16.25 |
| ATOM | 4712 | C   | LEU | 1321 | 85.959 | 58.608 | 41.259 | 1.00 | 17.08 |
| ATOM | 4713 | O   | LEU | 1321 | 85.424 | 59.689 | 41.027 | 1.00 | 16.83 |
| ATOM | 4714 | N   | ARG | 1322 | 85.887 | 57.581 | 40.421 | 1.00 | 14.82 |
| ATOM | 4715 | CA  | ARG | 1322 | 85.071 | 57.654 | 39.216 | 1.00 | 14.44 |
| ATOM | 4716 | CB  | ARG | 1322 | 85.820 | 57.032 | 38.043 | 1.00 | 11.02 |
| ATOM | 4717 | CG  | ARG | 1322 | 85.147 | 57.239 | 36.713 | 1.00 | 13.22 |
| ATOM | 4718 | CD  | ARG | 1322 | 86.089 | 56.862 | 35.596 | 1.00 | 14.14 |
| ATOM | 4719 | NE  | ARG | 1322 | 85.437 | 56.859 | 34.295 | 1.00 | 16.06 |
| ATOM | 4720 | CZ  | ARG | 1322 | 85.739 | 56.013 | 33.312 | 1.00 | 18.68 |
| ATOM | 4721 | NH1 | ARG | 1322 | 86.688 | 55.103 | 33.430 | 1.00 | 12.90 |
| ATOM | 4722 | NH2 | ARG | 1322 | 85.089 | 56.065 | 32.160 | 1.00 | 22.89 |
| ATOM | 4723 | C   | ARG | 1322 | 83.788 | 56.877 | 39.565 | 1.00 | 15.81 |
| ATOM | 4724 | O   | ARG | 1322 | 83.828 | 55.671 | 39.806 | 1.00 | 15.90 |
| ATOM | 4725 | N   | VAL | 1323 | 82.666 | 57.583 | 39.648 | 1.00 | 15.81 |
| ATOM | 4726 | CA  | VAL | 1323 | 81.407 | 56.972 | 40.047 | 1.00 | 16.05 |
| ATOM | 4727 | CB  | VAL | 1323 | 80.766 | 57.791 | 41.177 | 1.00 | 15.65 |
| ATOM | 4728 | CG1 | VAL | 1323 | 79.392 | 57.253 | 41.525 | 1.00 | 19.48 |
| ATOM | 4729 | CG2 | VAL | 1323 | 81.676 | 57.789 | 42.396 | 1.00 | 16.93 |
| ATOM | 4730 | C   | VAL | 1323 | 80.368 | 56.743 | 38.961 | 1.00 | 18.35 |
| ATOM | 4731 | O   | VAL | 1323 | 79.986 | 57.670 | 38.238 | 1.00 | 19.74 |
| ATOM | 4732 | N   | GLY | 1324 | 79.864 | 55.514 | 38.903 | 1.00 | 17.75 |
| ATOM | 4733 | CA  | GLY | 1324 | 78.850 | 55.170 | 37.927 | 1.00 | 15.53 |
| ATOM | 4734 | C   | GLY | 1324 | 78.957 | 53.738 | 37.447 | 1.00 | 15.75 |
| ATOM | 4735 | O   | GLY | 1324 | 80.061 | 53.250 | 37.213 | 1.00 | 16.50 |
| ATOM | 4736 | N   | MET | 1325 | 77.828 | 53.032 | 37.409 | 1.00 | 15.15 |
| ATOM | 4737 | CA  | MET | 1325 | 77.793 | 51.668 | 36.902 | 1.00 | 14.24 |
| ATOM | 4738 | CB  | MET | 1325 | 77.998 | 50.635 | 37.999 | 1.00 | 13.83 |
| ATOM | 4739 | CG  | MET | 1325 | 78.194 | 49.236 | 37.432 | 1.00 | 18.02 |
| ATOM | 4740 | SD  | MET | 1325 | 78.376 | 47.970 | 38.682 | 1.00 | 25.48 |
| ATOM | 4741 | CE  | MET | 1325 | 79.669 | 48.707 | 39.673 | 1.00 | 29.99 |
| ATOM | 4742 | C   | MET | 1325 | 76.496 | 51.387 | 36.140 | 1.00 | 13.62 |
| ATOM | 4743 | O   | MET | 1325 | 75.433 | 51.229 | 36.732 | 1.00 | 14.65 |
| ATOM | 4744 | N   | GLY | 1326 | 76.592 | 51.401 | 34.816 | 1.00 | 15.59 |
| ATOM | 4745 | CA  | GLY | 1326 | 75.449 | 51.129 | 33.968 | 1.00 | 18.92 |
| ATOM | 4746 | C   | GLY | 1326 | 74.629 | 52.296 | 33.448 | 1.00 | 21.59 |
| ATOM | 4747 | O   | GLY | 1326 | 73.781 | 52.111 | 32.576 | 1.00 | 23.28 |
| ATOM | 4748 | N   | CYS | 1327 | 74.872 | 53.496 | 33.954 | 1.00 | 23.19 |
| ATOM | 4749 | CA  | CYS | 1327 | 74.110 | 54.665 | 33.521 | 1.00 | 23.22 |
| ATOM | 4750 | CB  | CYS | 1327 | 74.136 | 55.729 | 34.613 | 1.00 | 18.50 |
| ATOM | 4751 | SG  | CYS | 1327 | 75.784 | 56.191 | 35.112 | 1.00 | 18.84 |
| ATOM | 4752 | C   | CYS | 1327 | 74.565 | 55.266 | 32.189 | 1.00 | 24.78 |
| ATOM | 4753 | O   | CYS | 1327 | 73.901 | 56.161 | 31.646 | 1.00 | 26.13 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 4870 | NH1 | ARG | 1341 | 74.766 | 53.690 | 46.412 | 1.00 | 3.80  |
| ATOM | 4871 | NH2 | ARG | 1341 | 72.593 | 53.820 | 47.128 | 1.00 | 3.16  |
| ATOM | 4872 | C   | ARG | 1341 | 72.579 | 53.009 | 39.660 | 1.00 | 10.77 |
| ATOM | 4873 | O   | ARG | 1341 | 73.217 | 53.550 | 38.753 | 1.00 | 11.78 |
| ATOM | 4874 | N   | PRO | 1342 | 71.383 | 53.481 | 40.069 | 1.00 | 10.84 |
| ATOM | 4875 | CD  | PRO | 1342 | 70.343 | 52.728 | 40.802 | 1.00 | 9.90  |
| ATOM | 4876 | CA  | PRO | 1342 | 70.840 | 54.746 | 39.568 | 1.00 | 10.04 |
| ATOM | 4877 | CB  | PRO | 1342 | 69.528 | 54.864 | 40.324 | 1.00 | 11.35 |
| ATOM | 4878 | CG  | PRO | 1342 | 69.078 | 53.444 | 40.408 | 1.00 | 8.27  |
| ATOM | 4879 | C   | PRO | 1342 | 71.822 | 55.876 | 39.908 | 1.00 | 12.01 |
| ATOM | 4880 | O   | PRO | 1342 | 72.144 | 56.118 | 41.080 | 1.00 | 14.18 |
| ATOM | 4881 | N   | GLN | 1343 | 72.267 | 56.583 | 38.877 | 1.00 | 12.98 |
| ATOM | 4882 | CA  | GLN | 1343 | 73.258 | 57.645 | 39.005 | 1.00 | 13.22 |
| ATOM | 4883 | CB  | GLN | 1343 | 73.562 | 58.248 | 37.630 | 1.00 | 11.87 |
| ATOM | 4884 | CG  | GLN | 1343 | 74.898 | 58.969 | 37.559 | 1.00 | 15.91 |
| ATOM | 4885 | CD  | GLN | 1343 | 76.076 | 58.115 | 38.015 | 1.00 | 20.74 |
| ATOM | 4886 | OE1 | GLN | 1343 | 75.935 | 56.919 | 38.293 | 1.00 | 23.33 |
| ATOM | 4887 | NE2 | GLN | 1343 | 77.247 | 58.730 | 38.090 | 1.00 | 21.84 |
| ATOM | 4888 | C   | GLN | 1343 | 73.132 | 58.742 | 40.060 | 1.00 | 14.18 |
| ATOM | 4889 | O   | GLN | 1343 | 74.038 | 58.911 | 40.867 | 1.00 | 16.74 |
| ATOM | 4890 | N   | ALA | 1344 | 72.052 | 59.512 | 40.064 | 1.00 | 14.34 |
| ATOM | 4891 | CA  | ALA | 1344 | 71.940 | 60.572 | 41.062 | 1.00 | 14.79 |
| ATOM | 4892 | CB  | ALA | 1344 | 70.638 | 61.304 | 40.927 | 1.00 | 14.45 |
| ATOM | 4893 | C   | ALA | 1344 | 72.086 | 60.012 | 42.466 | 1.00 | 15.98 |
| ATOM | 4894 | O   | ALA | 1344 | 72.612 | 60.685 | 43.351 | 1.00 | 18.86 |
| ATOM | 4895 | N   | THR | 1345 | 71.632 | 58.775 | 42.664 | 1.00 | 17.15 |
| ATOM | 4896 | CA  | THR | 1345 | 71.724 | 58.118 | 43.965 | 1.00 | 17.05 |
| ATOM | 4897 | CB  | THR | 1345 | 70.834 | 56.859 | 44.039 | 1.00 | 15.53 |
| ATOM | 4898 | OG1 | THR | 1345 | 69.452 | 57.234 | 43.996 | 1.00 | 13.75 |
| ATOM | 4899 | CG2 | THR | 1345 | 71.101 | 56.095 | 45.329 | 1.00 | 12.86 |
| ATOM | 4900 | C   | THR | 1345 | 73.168 | 57.734 | 44.284 | 1.00 | 17.66 |
| ATOM | 4901 | O   | THR | 1345 | 73.638 | 57.958 | 45.402 | 1.00 | 18.39 |
| ATOM | 4902 | N   | ALA | 1346 | 73.861 | 57.151 | 43.304 | 1.00 | 16.69 |
| ATOM | 4903 | CA  | ALA | 1346 | 75.257 | 56.738 | 43.478 | 1.00 | 14.38 |
| ATOM | 4904 | CB  | ALA | 1346 | 75.737 | 55.973 | 42.253 | 1.00 | 11.74 |
| ATOM | 4905 | C   | ALA | 1346 | 76.139 | 57.959 | 43.716 | 1.00 | 13.89 |
| ATOM | 4906 | O   | ALA | 1346 | 77.034 | 57.947 | 44.562 | 1.00 | 15.03 |
| ATOM | 4907 | N   | VAL | 1347 | 75.858 | 59.022 | 42.977 | 1.00 | 13.19 |
| ATOM | 4908 | CA  | VAL | 1347 | 76.610 | 60.255 | 43.098 | 1.00 | 13.37 |
| ATOM | 4909 | CB  | VAL | 1347 | 76.216 | 61.260 | 41.994 | 1.00 | 10.97 |
| ATOM | 4910 | CG1 | VAL | 1347 | 76.915 | 62.601 | 42.199 | 1.00 | 7.46  |
| ATOM | 4911 | CG2 | VAL | 1347 | 76.578 | 60.679 | 40.638 | 1.00 | 7.82  |
| ATOM | 4912 | C   | VAL | 1347 | 76.419 | 60.852 | 44.488 | 1.00 | 15.39 |
| ATOM | 4913 | O   | VAL | 1347 | 77.404 | 61.225 | 45.133 | 1.00 | 18.76 |
| ATOM | 4914 | N   | TYR | 1348 | 75.179 | 60.893 | 44.979 | 1.00 | 15.23 |
| ATOM | 4915 | CA  | TYR | 1348 | 74.927 | 61.441 | 46.311 | 1.00 | 15.80 |
| ATOM | 4916 | CB  | TYR | 1348 | 73.428 | 61.571 | 46.601 | 1.00 | 11.70 |
| ATOM | 4917 | CG  | TYR | 1348 | 73.169 | 62.031 | 48.018 | 1.00 | 11.19 |
| ATOM | 4918 | CD1 | TYR | 1348 | 73.374 | 63.354 | 48.383 | 1.00 | 13.82 |
| ATOM | 4919 | CE1 | TYR | 1348 | 73.219 | 63.775 | 49.704 | 1.00 | 12.58 |
| ATOM | 4920 | CD2 | TYR | 1348 | 72.792 | 61.132 | 49.014 | 1.00 | 13.36 |
| ATOM | 4921 | CE2 | TYR | 1348 | 72.633 | 61.545 | 50.341 | 1.00 | 11.68 |
| ATOM | 4922 | CZ  | TYR | 1348 | 72.850 | 62.872 | 50.672 | 1.00 | 12.94 |
| ATOM | 4923 | OH  | TYR | 1348 | 72.686 | 63.308 | 51.965 | 1.00 | 18.66 |
| ATOM | 4924 | C   | TYR | 1348 | 75.580 | 60.593 | 47.409 | 1.00 | 17.42 |
| ATOM | 4925 | O   | TYR | 1348 | 76.324 | 61.106 | 48.259 | 1.00 | 16.32 |
| ATOM | 4926 | N   | LYS | 1349 | 75.312 | 59.291 | 47.369 | 1.00 | 18.79 |
| ATOM | 4927 | CA  | LYS | 1349 | 75.838 | 58.352 | 48.357 | 1.00 | 20.46 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 4986 | CA  | ARG | 1356 | 85.020 | 62.575 | 54.610 | 1.00 | 25.43 |
| ATOM | 4987 | CB  | ARG | 1356 | 84.189 | 61.540 | 55.386 | 1.00 | 26.45 |
| ATOM | 4988 | CG  | ARG | 1356 | 82.714 | 61.888 | 55.487 | 1.00 | 33.21 |
| ATOM | 4989 | CD  | ARG | 1356 | 81.948 | 60.892 | 56.336 | 1.00 | 37.91 |
| ATOM | 4990 | NE  | ARG | 1356 | 80.540 | 61.270 | 56.459 | 1.00 | 44.13 |
| ATOM | 4991 | CZ  | ARG | 1356 | 80.064 | 62.180 | 57.311 | 1.00 | 50.10 |
| ATOM | 4992 | NH1 | ARG | 1356 | 80.876 | 62.829 | 58.142 | 1.00 | 50.72 |
| ATOM | 4993 | NH2 | ARG | 1356 | 78.765 | 62.456 | 57.327 | 1.00 | 51.78 |
| ATOM | 4994 | C   | ARG | 1356 | 86.505 | 62.167 | 54.580 | 1.00 | 24.79 |
| ATOM | 4995 | O   | ARG | 1356 | 87.144 | 62.017 | 55.626 | 1.00 | 28.39 |
| ATOM | 4996 | N   | PHE | 1357 | 87.053 | 62.006 | 53.380 | 1.00 | 20.35 |
| ATOM | 4997 | CA  | PHE | 1357 | 88.440 | 61.617 | 53.214 | 1.00 | 19.19 |
| ATOM | 4998 | CB  | PHE | 1357 | 88.495 | 60.141 | 52.842 | 1.00 | 18.36 |
| ATOM | 4999 | CG  | PHE | 1357 | 87.699 | 59.288 | 53.765 | 1.00 | 19.85 |
| ATOM | 5000 | CD1 | PHE | 1357 | 88.239 | 58.871 | 54.978 | 1.00 | 21.81 |
| ATOM | 5001 | CD2 | PHE | 1357 | 86.367 | 59.018 | 53.499 | 1.00 | 19.20 |
| ATOM | 5002 | CE1 | PHE | 1357 | 87.456 | 56.211 | 55.919 | 1.00 | 18.86 |
| ATOM | 5003 | CE2 | PHE | 1357 | 85.583 | 58.362 | 54.432 | 1.00 | 20.85 |
| ATOM | 5004 | CZ  | PHE | 1357 | 86.129 | 57.960 | 55.646 | 1.00 | 18.81 |
| ATOM | 5005 | C   | PHE | 1357 | 89.113 | 62.473 | 52.158 | 1.00 | 20.97 |
| ATOM | 5006 | O   | PHE | 1357 | 90.140 | 62.092 | 51.590 | 1.00 | 22.54 |
| ATOM | 5007 | N   | GLY | 1358 | 88.509 | 63.626 | 51.884 | 1.00 | 20.40 |
| ATOM | 5008 | CA  | GLY | 1358 | 89.043 | 64.549 | 50.899 | 1.00 | 17.74 |
| ATOM | 5009 | C   | GLY | 1358 | 89.167 | 63.989 | 49.498 | 1.00 | 17.67 |
| ATOM | 5010 | O   | GLY | 1358 | 89.860 | 64.575 | 48.660 | 1.00 | 19.43 |
| ATOM | 5011 | N   | VAL | 1359 | 88.485 | 62.883 | 49.221 | 1.00 | 15.95 |
| ATOM | 5012 | CA  | VAL | 1359 | 88.562 | 62.270 | 47.902 | 1.00 | 15.11 |
| ATOM | 5013 | CB  | VAL | 1359 | 88.490 | 60.742 | 47.991 | 1.00 | 11.79 |
| ATOM | 5014 | CG1 | VAL | 1359 | 88.597 | 60.139 | 46.612 | 1.00 | 12.33 |
| ATOM | 5015 | CG2 | VAL | 1359 | 89.604 | 60.219 | 48.871 | 1.00 | 13.37 |
| ATOM | 5016 | C   | VAL | 1359 | 87.455 | 62.766 | 46.976 | 1.00 | 15.32 |
| ATOM | 5017 | O   | VAL | 1359 | 86.276 | 62.506 | 47.213 | 1.00 | 16.23 |
| ATOM | 5018 | N   | PRO | 1360 | 87.823 | 63.527 | 45.933 | 1.00 | 15.11 |
| ATOM | 5019 | CD  | PRO | 1360 | 89.158 | 64.109 | 45.719 | 1.00 | 14.19 |
| ATOM | 5020 | CA  | PRO | 1360 | 86.871 | 64.067 | 44.960 | 1.00 | 15.11 |
| ATOM | 5021 | CB  | PRO | 1360 | 87.766 | 64.902 | 44.047 | 1.00 | 15.19 |
| ATOM | 5022 | CG  | PRO | 1360 | 88.832 | 65.371 | 44.977 | 1.00 | 12.72 |
| ATOM | 5023 | C   | PRO | 1360 | 86.138 | 62.962 | 44.195 | 1.00 | 14.73 |
| ATOM | 5024 | O   | PRO | 1360 | 86.675 | 61.875 | 43.995 | 1.00 | 15.41 |
| ATOM | 5025 | N   | VAL | 1361 | 84.919 | 63.262 | 43.756 | 1.00 | 14.39 |
| ATOM | 5026 | CA  | VAL | 1361 | 84.074 | 62.311 | 43.048 | 1.00 | 13.41 |
| ATOM | 5027 | CB  | VAL | 1361 | 82.783 | 62.027 | 43.881 | 1.00 | 12.70 |
| ATOM | 5028 | CG1 | VAL | 1361 | 81.633 | 61.550 | 43.000 | 1.00 | 11.96 |
| ATOM | 5029 | CG2 | VAL | 1361 | 83.084 | 60.991 | 44.951 | 1.00 | 11.77 |
| ATOM | 5030 | C   | VAL | 1361 | 83.703 | 62.786 | 41.647 | 1.00 | 13.98 |
| ATOM | 5031 | O   | VAL | 1361 | 83.104 | 63.845 | 41.483 | 1.00 | 14.14 |
| ATOM | 5032 | N   | ILE | 1362 | 84.069 | 61.991 | 40.647 | 1.00 | 15.72 |
| ATOM | 5033 | CA  | ILE | 1362 | 83.770 | 62.280 | 39.244 | 1.00 | 17.31 |
| ATOM | 5034 | CB  | ILE | 1362 | 84.853 | 61.691 | 38.273 | 1.00 | 15.17 |
| ATOM | 5035 | CG2 | ILE | 1362 | 84.462 | 61.952 | 36.822 | 1.00 | 7.15  |
| ATOM | 5036 | CG1 | ILE | 1362 | 86.246 | 62.259 | 38.587 | 1.00 | 15.08 |
| ATOM | 5037 | CD1 | ILE | 1362 | 87.343 | 61.761 | 37.659 | 1.00 | 5.33  |
| ATOM | 5038 | C   | ILE | 1362 | 82.452 | 61.584 | 38.917 | 1.00 | 19.48 |
| ATOM | 5039 | O   | ILE | 1362 | 82.396 | 60.348 | 38.906 | 1.00 | 20.54 |
| ATOM | 5040 | N   | ALA | 1363 | 81.393 | 62.363 | 38.685 | 1.00 | 19.94 |
| ATOM | 5041 | CA  | ALA | 1363 | 80.082 | 61.807 | 38.337 | 1.00 | 18.31 |
| ATOM | 5042 | CB  | ALA | 1363 | 78.996 | 62.841 | 38.555 | 1.00 | 17.29 |
| ATOM | 5043 | C   | ALA | 1363 | 80.158 | 61.387 | 36.869 | 1.00 | 18.95 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5044 | O   | ALA | 1363 | 80.061 | 62.218 | 35.961 | 1.00 | 17.38 |
| ATOM | 5045 | N   | ASP | 1364 | 80.309 | 60.083 | 36.656 | 1.00 | 21.34 |
| ATOM | 5046 | CA  | ASP | 1364 | 80.484 | 59.502 | 35.327 | 1.00 | 22.87 |
| ATOM | 5047 | CB  | ASP | 1364 | 81.804 | 58.715 | 35.345 | 1.00 | 22.78 |
| ATOM | 5048 | CG  | ASP | 1364 | 82.068 | 57.973 | 34.065 | 1.00 | 19.89 |
| ATOM | 5049 | OD1 | ASP | 1364 | 81.786 | 58.524 | 32.990 | 1.00 | 18.84 |
| ATOM | 5050 | OD2 | ASP | 1364 | 82.571 | 56.838 | 34.139 | 1.00 | 22.02 |
| ATOM | 5051 | C   | ASP | 1364 | 79.354 | 58.638 | 34.739 | 1.00 | 22.91 |
| ATOM | 5052 | O   | ASP | 1364 | 79.172 | 57.479 | 35.123 | 1.00 | 22.90 |
| ATOM | 5053 | N   | GLY | 1365 | 78.675 | 59.179 | 33.731 | 1.00 | 22.55 |
| ATOM | 5054 | CA  | GLY | 1365 | 77.601 | 58.453 | 33.081 | 1.00 | 22.28 |
| ATOM | 5055 | C   | GLY | 1365 | 76.211 | 59.013 | 33.325 | 1.00 | 22.48 |
| ATOM | 5056 | O   | GLY | 1365 | 75.886 | 59.417 | 34.439 | 1.00 | 22.82 |
| ATOM | 5057 | N   | GLY | 1366 | 75.398 | 59.047 | 32.272 | 1.00 | 23.81 |
| ATOM | 5058 | CA  | GLY | 1366 | 74.037 | 59.540 | 32.383 | 1.00 | 25.79 |
| ATOM | 5059 | C   | GLY | 1366 | 73.820 | 61.032 | 32.203 | 1.00 | 27.55 |
| ATOM | 5060 | O   | GLY | 1366 | 72.827 | 61.578 | 32.678 | 1.00 | 30.08 |
| ATOM | 5061 | N   | ILE | 1367 | 74.742 | 61.711 | 31.536 | 1.00 | 29.05 |
| ATOM | 5062 | CA  | ILE | 1367 | 74.600 | 63.139 | 31.305 | 1.00 | 28.73 |
| ATOM | 5063 | CB  | ILE | 1367 | 75.948 | 63.897 | 31.486 | 1.00 | 29.81 |
| ATOM | 5064 | CG2 | ILE | 1367 | 75.757 | 65.397 | 31.255 | 1.00 | 29.11 |
| ATOM | 5065 | CG1 | ILE | 1367 | 76.546 | 63.631 | 32.873 | 1.00 | 28.67 |
| ATOM | 5066 | CD1 | ILE | 1367 | 75.734 | 64.175 | 34.022 | 1.00 | 28.35 |
| ATOM | 5067 | C   | ILE | 1367 | 74.138 | 63.310 | 29.862 | 1.00 | 30.48 |
| ATOM | 5068 | O   | ILE | 1367 | 74.561 | 62.565 | 28.969 | 1.00 | 31.42 |
| ATOM | 5069 | N   | GLN | 1368 | 73.237 | 64.261 | 29.645 | 1.00 | 31.28 |
| ATOM | 5070 | CA  | GLN | 1368 | 72.734 | 64.561 | 28.308 | 1.00 | 33.21 |
| ATOM | 5071 | CB  | GLN | 1368 | 71.673 | 63.558 | 27.850 | 1.00 | 38.74 |
| ATOM | 5072 | CG  | GLN | 1368 | 72.188 | 62.559 | 26.791 | 1.00 | 47.07 |
| ATOM | 5073 | CD  | GLN | 1368 | 72.526 | 63.203 | 25.434 | 1.00 | 49.78 |
| ATOM | 5074 | OE1 | GLN | 1368 | 71.694 | 63.239 | 24.523 | 1.00 | 51.57 |
| ATOM | 5075 | NE2 | GLN | 1368 | 73.759 | 63.666 | 25.287 | 1.00 | 49.82 |
| ATOM | 5076 | C   | GLN | 1368 | 72.217 | 65.984 | 28.212 | 1.00 | 31.65 |
| ATOM | 5077 | O   | GLN | 1368 | 71.541 | 66.347 | 27.258 | 1.00 | 33.54 |
| ATOM | 5078 | N   | ASN | 1369 | 72.551 | 66.786 | 29.213 | 1.00 | 28.87 |
| ATOM | 5079 | CA  | ASN | 1369 | 72.176 | 68.185 | 29.253 | 1.00 | 27.68 |
| ATOM | 5080 | CB  | ASN | 1369 | 70.650 | 68.398 | 29.193 | 1.00 | 26.97 |
| ATOM | 5081 | CG  | ASN | 1369 | 69.903 | 67.728 | 30.324 | 1.00 | 26.85 |
| ATOM | 5082 | OD1 | ASN | 1369 | 70.263 | 67.852 | 31.496 | 1.00 | 26.95 |
| ATOM | 5083 | ND2 | ASN | 1369 | 68.829 | 67.037 | 29.978 | 1.00 | 28.12 |
| ATOM | 5084 | C   | ASN | 1369 | 72.782 | 68.803 | 30.494 | 1.00 | 27.65 |
| ATOM | 5085 | O   | ASN | 1369 | 73.240 | 68.082 | 31.396 | 1.00 | 27.37 |
| ATOM | 5086 | N   | VAL | 1370 | 72.844 | 70.133 | 30.497 | 1.00 | 26.63 |
| ATOM | 5087 | CA  | VAL | 1370 | 73.404 | 70.901 | 31.601 | 1.00 | 23.97 |
| ATOM | 5088 | CB  | VAL | 1370 | 73.319 | 72.421 | 31.311 | 1.00 | 25.11 |
| ATOM | 5089 | CG1 | VAL | 1370 | 73.858 | 73.222 | 32.487 | 1.00 | 25.59 |
| ATOM | 5090 | CG2 | VAL | 1370 | 74.089 | 72.758 | 30.038 | 1.00 | 18.81 |
| ATOM | 5091 | C   | VAL | 1370 | 72.684 | 70.569 | 32.902 | 1.00 | 22.46 |
| ATOM | 5092 | O   | VAL | 1370 | 73.298 | 70.540 | 33.967 | 1.00 | 21.96 |
| ATOM | 5093 | N   | GLY | 1371 | 71.389 | 70.285 | 32.799 | 1.00 | 22.70 |
| ATOM | 5094 | CA  | GLY | 1371 | 70.599 | 69.939 | 33.968 | 1.00 | 20.55 |
| ATOM | 5095 | C   | GLY | 1371 | 71.251 | 68.798 | 34.714 | 1.00 | 19.42 |
| ATOM | 5096 | O   | GLY | 1371 | 71.468 | 68.881 | 35.914 | 1.00 | 20.90 |
| ATOM | 5097 | N   | HIS | 1372 | 71.613 | 67.746 | 33.993 | 1.00 | 18.46 |
| ATOM | 5098 | CA  | HIS | 1372 | 72.260 | 66.596 | 34.600 | 1.00 | 17.54 |
| ATOM | 5099 | CB  | HIS | 1372 | 72.555 | 65.532 | 33.538 | 1.00 | 19.84 |
| ATOM | 5100 | CG  | HIS | 1372 | 71.327 | 64.935 | 32.917 | 1.00 | 19.86 |
| ATOM | 5101 | CD2 | HIS | 1372 | 71.148 | 64.297 | 31.733 | 1.00 | 16.94 |



FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5102 | ND1 | HIS | 1372 | 70.099 | 64.914 | 33.540 | 1.00 | 20.56 |
| ATOM | 5103 | CE1 | HIS | 1372 | 69.222 | 64.291 | 32.779 | 1.00 | 18.07 |
| ATOM | 5104 | NE2 | HIS | 1372 | 69.841 | 63.907 | 31.674 | 1.00 | 18.04 |
| ATOM | 5105 | C   | HIS | 1372 | 73.556 | 67.024 | 35.287 | 1.00 | 16.89 |
| ATOM | 5106 | O   | HIS | 1372 | 73.819 | 66.642 | 36.425 | 1.00 | 16.89 |
| ATOM | 5107 | N   | ILE | 1373 | 74.337 | 67.860 | 34.610 | 1.00 | 17.42 |
| ATOM | 5108 | CA  | ILE | 1373 | 75.606 | 68.341 | 35.154 | 1.00 | 15.96 |
| ATOM | 5109 | CB  | ILE | 1373 | 76.362 | 69.204 | 34.134 | 1.00 | 15.20 |
| ATOM | 5110 | CG2 | ILE | 1373 | 77.651 | 69.733 | 34.743 | 1.00 | 17.65 |
| ATOM | 5111 | CG1 | ILE | 1373 | 76.666 | 68.381 | 32.880 | 1.00 | 9.89  |
| ATOM | 5112 | CD1 | ILE | 1373 | 77.325 | 69.185 | 31.795 | 1.00 | 8.53  |
| ATOM | 5113 | C   | ILE | 1373 | 75.433 | 69.121 | 36.456 | 1.00 | 15.25 |
| ATOM | 5114 | O   | ILE | 1373 | 76.138 | 68.863 | 37.430 | 1.00 | 16.51 |
| ATOM | 5115 | N   | ALA | 1374 | 74.498 | 70.065 | 36.477 | 1.00 | 14.86 |
| ATOM | 5116 | CA  | ALA | 1374 | 74.235 | 70.854 | 37.679 | 1.00 | 14.25 |
| ATOM | 5117 | CB  | ALA | 1374 | 73.204 | 71.923 | 37.394 | 1.00 | 11.74 |
| ATOM | 5118 | C   | ALA | 1374 | 73.758 | 69.963 | 38.823 | 1.00 | 15.36 |
| ATOM | 5119 | O   | ALA | 1374 | 74.166 | 70.146 | 39.967 | 1.00 | 16.74 |
| ATOM | 5120 | N   | LYS | 1375 | 72.923 | 68.977 | 38.506 | 1.00 | 16.36 |
| ATOM | 5121 | CA  | LYS | 1375 | 72.390 | 68.063 | 39.515 | 1.00 | 16.18 |
| ATOM | 5122 | CB  | LYS | 1375 | 71.293 | 67.177 | 38.921 | 1.00 | 16.44 |
| ATOM | 5123 | CG  | LYS | 1375 | 70.020 | 67.950 | 38.597 | 1.00 | 16.99 |
| ATOM | 5124 | CD  | LYS | 1375 | 68.973 | 67.103 | 37.894 | 1.00 | 17.81 |
| ATOM | 5125 | CE  | LYS | 1375 | 67.701 | 67.914 | 37.671 | 1.00 | 18.59 |
| ATOM | 5126 | NZ  | LYS | 1375 | 66.576 | 67.092 | 37.162 | 1.00 | 16.68 |
| ATOM | 5127 | C   | LYS | 1375 | 73.484 | 67.219 | 40.137 | 1.00 | 15.85 |
| ATOM | 5128 | O   | LYS | 1375 | 73.546 | 67.080 | 41.359 | 1.00 | 16.57 |
| ATOM | 5129 | N   | ALA | 1376 | 74.357 | 66.672 | 39.300 | 1.00 | 14.84 |
| ATOM | 5130 | CA  | ALA | 1376 | 75.468 | 65.867 | 39.786 | 1.00 | 13.60 |
| ATOM | 5131 | CB  | ALA | 1376 | 76.314 | 65.398 | 38.633 | 1.00 | 11.96 |
| ATOM | 5132 | C   | ALA | 1376 | 76.309 | 66.714 | 40.732 | 1.00 | 14.60 |
| ATOM | 5133 | O   | ALA | 1376 | 76.601 | 66.300 | 41.849 | 1.00 | 17.56 |
| ATOM | 5134 | N   | LEU | 1377 | 76.661 | 67.918 | 40.295 | 1.00 | 13.87 |
| ATOM | 5135 | CA  | LEU | 1377 | 77.466 | 68.829 | 41.100 | 1.00 | 14.63 |
| ATOM | 5136 | CB  | LEU | 1377 | 77.741 | 70.126 | 40.322 | 1.00 | 14.18 |
| ATOM | 5137 | CG  | LEU | 1377 | 78.412 | 70.033 | 38.945 | 1.00 | 11.92 |
| ATOM | 5138 | CD1 | LEU | 1377 | 78.385 | 71.376 | 38.281 | 1.00 | 11.93 |
| ATOM | 5139 | CD2 | LEU | 1377 | 79.831 | 69.521 | 39.049 | 1.00 | 10.66 |
| ATOM | 5140 | C   | LEU | 1377 | 76.728 | 69.155 | 42.394 | 1.00 | 15.88 |
| ATOM | 5141 | O   | LEU | 1377 | 77.289 | 69.070 | 43.482 | 1.00 | 16.02 |
| ATOM | 5142 | N   | ALA | 1378 | 75.442 | 69.460 | 42.266 | 1.00 | 18.34 |
| ATOM | 5143 | CA  | ALA | 1378 | 74.606 | 69.813 | 43.406 | 1.00 | 18.74 |
| ATOM | 5144 | CB  | ALA | 1378 | 73.235 | 70.252 | 42.931 | 1.00 | 18.93 |
| ATOM | 5145 | C   | ALA | 1378 | 74.474 | 68.688 | 44.414 | 1.00 | 20.05 |
| ATOM | 5146 | O   | ALA | 1378 | 74.233 | 68.927 | 45.600 | 1.00 | 23.62 |
| ATOM | 5147 | N   | LEU | 1379 | 74.631 | 67.456 | 43.957 | 1.00 | 19.27 |
| ATOM | 5148 | CA  | LEU | 1379 | 74.514 | 66.330 | 44.862 | 1.00 | 17.31 |
| ATOM | 5149 | CB  | LEU | 1379 | 73.839 | 65.160 | 44.158 | 1.00 | 14.86 |
| ATOM | 5150 | CG  | LEU | 1379 | 72.367 | 65.373 | 43.794 | 1.00 | 11.16 |
| ATOM | 5151 | CD1 | LEU | 1379 | 71.828 | 64.139 | 43.131 | 1.00 | 13.25 |
| ATOM | 5152 | CD2 | LEU | 1379 | 71.563 | 65.666 | 45.038 | 1.00 | 12.87 |
| ATOM | 5153 | C   | LEU | 1379 | 75.820 | 65.902 | 45.530 | 1.00 | 19.22 |
| ATOM | 5154 | O   | LEU | 1379 | 75.799 | 65.039 | 46.406 | 1.00 | 22.97 |
| ATOM | 5155 | N   | GLY | 1380 | 76.951 | 66.490 | 45.137 | 1.00 | 18.29 |
| ATOM | 5156 | CA  | GLY | 1380 | 78.210 | 66.122 | 45.773 | 1.00 | 18.10 |
| ATOM | 5157 | C   | GLY | 1380 | 79.440 | 65.888 | 44.907 | 1.00 | 17.70 |
| ATOM | 5158 | O   | GLY | 1380 | 80.567 | 66.032 | 45.380 | 1.00 | 14.69 |
| ATOM | 5159 | N   | ALA | 1381 | 79.240 | 65.501 | 43.653 | 1.00 | 18.38 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5160 | CA  | ALA | 1381 | 80.359 | 65.247 | 42.753 | 1.00 | 18.79 |
| ATOM | 5161 | CB  | ALA | 1381 | 79.849 | 64.746 | 41.422 | 1.00 | 17.88 |
| ATOM | 5162 | C   | ALA | 1381 | 81.179 | 66.507 | 42.545 | 1.00 | 19.77 |
| ATOM | 5163 | O   | ALA | 1381 | 80.628 | 67.601 | 42.532 | 1.00 | 22.90 |
| ATOM | 5164 | N   | SER | 1382 | 82.492 | 66.358 | 42.400 | 1.00 | 20.02 |
| ATOM | 5165 | CA  | SER | 1382 | 83.367 | 67.507 | 42.160 | 1.00 | 20.59 |
| ATOM | 5166 | CB  | SER | 1382 | 84.749 | 67.266 | 42.768 | 1.00 | 18.13 |
| ATOM | 5167 | OG  | SER | 1382 | 84.652 | 67.191 | 44.180 | 1.00 | 15.75 |
| ATOM | 5168 | C   | SER | 1382 | 83.475 | 67.871 | 40.668 | 1.00 | 20.80 |
| ATOM | 5169 | O   | SER | 1382 | 83.501 | 69.054 | 40.304 | 1.00 | 21.81 |
| ATOM | 5170 | N   | THR | 1383 | 83.535 | 66.856 | 39.813 | 1.00 | 17.88 |
| ATOM | 5171 | CA  | THR | 1383 | 83.621 | 67.065 | 38.377 | 1.00 | 17.53 |
| ATOM | 5172 | CB  | THR | 1383 | 85.075 | 66.831 | 37.818 | 1.00 | 17.61 |
| ATOM | 5173 | OG1 | THR | 1383 | 85.611 | 65.603 | 38.328 | 1.00 | 20.84 |
| ATOM | 5174 | CG2 | THR | 1383 | 86.013 | 67.982 | 38.180 | 1.00 | 8.94  |
| ATOM | 5175 | C   | THR | 1383 | 82.639 | 66.100 | 37.719 | 1.00 | 17.87 |
| ATOM | 5176 | O   | THR | 1383 | 82.062 | 65.243 | 38.388 | 1.00 | 18.28 |
| ATOM | 5177 | N   | VAL | 1384 | 82.457 | 66.225 | 36.411 | 1.00 | 17.76 |
| ATOM | 5178 | CA  | VAL | 1384 | 81.531 | 65.370 | 35.689 | 1.00 | 18.85 |
| ATOM | 5179 | CB  | VAL | 1384 | 80.239 | 66.138 | 35.325 | 1.00 | 20.09 |
| ATOM | 5180 | CG1 | VAL | 1384 | 79.243 | 65.206 | 34.650 | 1.00 | 22.58 |
| ATOM | 5181 | CG2 | VAL | 1384 | 79.618 | 66.748 | 36.576 | 1.00 | 19.94 |
| ATOM | 5182 | C   | VAL | 1384 | 82.211 | 64.888 | 34.417 | 1.00 | 19.13 |
| ATOM | 5183 | O   | VAL | 1384 | 82.887 | 65.665 | 33.747 | 1.00 | 19.52 |
| ATOM | 5184 | N   | MET | 1385 | 82.044 | 63.606 | 34.104 | 1.00 | 19.13 |
| ATOM | 5185 | CA  | MET | 1385 | 82.645 | 62.997 | 32.915 | 1.00 | 18.23 |
| ATOM | 5186 | CB  | MET | 1385 | 83.345 | 61.688 | 33.284 | 1.00 | 17.04 |
| ATOM | 5187 | CG  | MET | 1385 | 84.081 | 61.051 | 32.136 | 1.00 | 13.46 |
| ATOM | 5188 | SD  | MET | 1385 | 84.923 | 59.571 | 32.655 | 1.00 | 19.09 |
| ATOM | 5189 | CE  | MET | 1385 | 86.456 | 60.251 | 33.317 | 1.00 | 21.08 |
| ATOM | 5190 | C   | MET | 1385 | 81.578 | 62.719 | 31.868 | 1.00 | 17.99 |
| ATOM | 5191 | O   | MET | 1385 | 80.519 | 62.179 | 32.182 | 1.00 | 19.60 |
| ATOM | 5192 | N   | MET | 1386 | 81.875 | 63.037 | 30.615 | 1.00 | 18.35 |
| ATOM | 5193 | CA  | MET | 1386 | 80.910 | 62.837 | 29.541 | 1.00 | 16.61 |
| ATOM | 5194 | CB  | MET | 1386 | 80.431 | 64.190 | 29.027 | 1.00 | 14.36 |
| ATOM | 5195 | CG  | MET | 1386 | 79.810 | 65.051 | 30.037 | 1.00 | 12.38 |
| ATOM | 5196 | SD  | MET | 1386 | 79.667 | 66.733 | 29.547 | 1.00 | 18.87 |
| ATOM | 5197 | CE  | MET | 1386 | 81.312 | 67.356 | 29.974 | 1.00 | 17.73 |
| ATOM | 5198 | C   | MET | 1386 | 81.441 | 62.023 | 28.376 | 1.00 | 15.70 |
| ATOM | 5199 | O   | MET | 1386 | 82.617 | 62.092 | 28.044 | 1.00 | 11.01 |
| ATOM | 5200 | N   | GLY | 1387 | 80.561 | 61.212 | 27.806 | 1.00 | 19.29 |
| ATOM | 5201 | CA  | GLY | 1387 | 80.901 | 60.398 | 26.659 | 1.00 | 23.41 |
| ATOM | 5202 | C   | GLY | 1387 | 80.052 | 60.931 | 25.523 | 1.00 | 26.99 |
| ATOM | 5203 | O   | GLY | 1387 | 80.526 | 61.715 | 24.698 | 1.00 | 29.23 |
| ATOM | 5204 | N   | SER | 1388 | 78.761 | 60.624 | 25.566 | 1.00 | 28.65 |
| ATOM | 5205 | CA  | SER | 1388 | 77.815 | 61.065 | 24.545 | 1.00 | 31.48 |
| ATOM | 5206 | CB  | SER | 1388 | 76.399 | 60.589 | 24.898 | 1.00 | 35.04 |
| ATOM | 5207 | OG  | SER | 1388 | 75.483 | 60.905 | 23.859 | 1.00 | 41.86 |
| ATOM | 5208 | C   | SER | 1388 | 77.803 | 62.578 | 24.284 | 1.00 | 31.07 |
| ATOM | 5209 | O   | SER | 1388 | 77.956 | 63.008 | 23.142 | 1.00 | 31.04 |
| ATOM | 5210 | N   | LEU | 1389 | 77.646 | 63.379 | 25.336 | 1.00 | 30.90 |
| ATOM | 5211 | CA  | LEU | 1389 | 77.599 | 64.835 | 25.204 | 1.00 | 29.63 |
| ATOM | 5212 | CB  | LEU | 1389 | 77.516 | 65.514 | 26.574 | 1.00 | 27.98 |
| ATOM | 5213 | CG  | LEU | 1389 | 76.164 | 66.067 | 27.033 | 1.00 | 28.79 |
| ATOM | 5214 | CD1 | LEU | 1389 | 76.373 | 67.062 | 28.167 | 1.00 | 26.81 |
| ATOM | 5215 | CD2 | LEU | 1389 | 75.460 | 66.758 | 25.889 | 1.00 | 28.61 |
| ATOM | 5216 | C   | LEU | 1389 | 78.762 | 65.450 | 24.438 | 1.00 | 30.59 |
| ATOM | 5217 | O   | LEU | 1389 | 78.662 | 66.588 | 23.989 | 1.00 | 33.45 |

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FIGURE 1 (CONT.)

|      |      |     |     |      |        |                     |        |      |       |
|------|------|-----|-----|------|--------|---------------------|--------|------|-------|
| ATOM | 5218 | N   | LEU | 1390 | 79.866 | 64.723              | 24.304 | 1.00 | 28.48 |
| ATOM | 5219 | CA  | LEU | 1390 | 81.030 | 65.247              | 23.601 | 1.00 | 26.24 |
| ATOM | 5220 | CB  | LEU | 1390 | 82.189 | 65.398              | 24.585 | 1.00 | 23.55 |
| ATOM | 5221 | CG  | LEU | 1390 | 81.834 | 66.123              | 25.890 | 1.00 | 23.78 |
| ATOM | 5222 | CD1 | LEU | 1390 | 82.978 | 66.032              | 26.883 | 1.00 | 24.77 |
| ATOM | 5223 | CD2 | LEU | 1390 | 81.467 | 67.578              | 25.614 | 1.00 | 20.41 |
| ATOM | 5224 | C   | LEU | 1390 | 81.427 | 64.325              | 22.456 | 1.00 | 27.34 |
| ATOM | 5225 | O   | LEU | 1390 | 82.375 | 64.599              | 21.727 | 1.00 | 26.38 |
| ATOM | 5226 | N   | ALA | 1391 | 80.642 | 63.270              | 22.265 | 1.00 | 29.15 |
| ATOM | 5227 | CA  | ALA | 1391 | 80.890 | 62.267              | 21.235 | 1.00 | 31.26 |
| ATOM | 5228 | CB  | ALA | 1391 | 79.927 | 61.100              | 21.404 | 1.00 | 31.73 |
| ATOM | 5229 | C   | ALA | 1391 | 80.903 | 62.719              | 19.777 | 1.00 | 32.50 |
| ATOM | 5230 | O   | ALA | 1391 | 81.734 | 62.250              | 18.998 | 1.00 | 35.88 |
| ATOM | 5231 | N   | ALA | 1392 | 79.975 | 63.585              | 19.383 | 1.00 | 30.95 |
| ATOM | 5232 | CA  | ALA | 1392 | 79.932 | 64.034              | 17.990 | 1.00 | 28.80 |
| ATOM | 5233 | CB  | ALA | 1392 | 78.504 | 64.045              | 17.489 | 1.00 | 28.83 |
| ATOM | 5234 | C   | ALA | 1392 | 80.576 | 65.393              | 17.754 | 1.00 | 27.78 |
| ATOM | 5235 | O   | ALA | 1392 | 80.169 | 66.121              | 16.849 | 1.00 | 28.88 |
| ATOM | 5236 | N   | THR | 1393 | 81.551 | 65.757              | 18.579 | 1.00 | 26.43 |
| ATOM | 5237 | CA  | THR | 1393 | 82.217 | 67.042              | 18.418 | 1.00 | 23.76 |
| ATOM | 5238 | CB  | THR | 1393 | 82.798 | 67.557              | 19.742 | 1.00 | 19.29 |
| ATOM | 5239 | OG1 | THR | 1393 | 83.646 | 66.563              | 20.316 | 1.00 | 20.30 |
| ATOM | 5240 | CG2 | THR | 1393 | 81.684 | 67.894              | 20.719 | 1.00 | 15.86 |
| ATOM | 5241 | C   | THR | 1393 | 83.323 | 66.910              | 17.373 | 1.00 | 24.72 |
| ATOM | 5242 | O   | THR | 1393 | 83.803 | 65.807              | 17.109 | 1.00 | 25.78 |
| ATOM | 5243 | N   | THR | 1394 | 83.735 | 68.032              | 16.795 | 1.00 | 23.33 |
| ATOM | 5244 | CA  | THR | 1394 | 84.761 | 68.036              | 15.767 | 1.00 | 22.70 |
| ATOM | 5245 | CB  | THR | 1394 | 85.078 | 69.469              | 15.314 | 1.00 | 22.05 |
| ATOM | 5246 | OG1 | THR | 1394 | 83.898 | 70.271              | 15.392 | 1.00 | 23.20 |
| ATOM | 5247 | CG2 | THR | 1394 | 85.552 | 69.468              | 13.882 | 1.00 | 23.82 |
| ATOM | 5248 | C   | THR | 1394 | 86.052 | 67.361              | 16.224 | 1.00 | 23.54 |
| ATOM | 5249 | O   | THR | 1394 | 86.690 | 66.643              | 15.448 | 1.00 | 24.72 |
| ATOM | 5250 | N   | GLU | 1395 | 86.409 | 67.566              | 17.490 | 1.00 | 22.73 |
| ATOM | 5251 | CA  | GLU | 1395 | 87.634 | 67.007              | 18.059 | 1.00 | 23.52 |
| ATOM | 5252 | CB  | GLU | 1395 | 88.078 | 67.819              | 19.283 | 1.00 | 25.10 |
| ATOM | 5253 | CG  | GLU | 1395 | 88.494 | 69.254              | 18.995 | 1.00 | 27.32 |
| ATOM | 5254 | CD  | GLU | 1395 | 87.322 | 70.185              | 18.752 | 1.00 | 31.55 |
| ATOM | 5255 | OE1 | GLU | 1395 | 86.177 | 69.833              | 19.102 | 1.00 | 34.70 |
| ATOM | 5256 | OE2 | GLU | 1395 | 87.547 | 71.287              | 18.216 | 1.00 | 35.64 |
| ATOM | 5257 | C   | GLU | 1395 | 87.560 | 65.536              | 18.460 | 1.00 | 23.45 |
| ATOM | 5258 | O   | GLU | 1395 | 88.578 | 64.936              | 18.817 | 1.00 | 26.40 |
| ATOM | 5259 | N   | ALA | 1396 | 86.367 | 64.966              | 18.462 | 1.00 | 22.70 |
| ATOM | 5260 | CA  | ALA | 1396 | 86.219 | 63.570              | 18.842 | 1.00 | 23.99 |
| ATOM | 5261 | CB  | ALA | 1396 | 84.743 | 63.219              | 18.969 | 1.00 | 23.65 |
| ATOM | 5262 | C   | ALA | 1396 | 86.880 | 62.703              | 17.779 | 1.00 | 25.22 |
| ATOM | 5263 | O   | ALA | 1396 | 86.920 | 63.081              | 16.611 | 1.00 | 26.43 |
| ATOM | 5264 | N   | PRO | 1397 | 87.487 | 61.570              | 18.184 | 1.00 | 25.84 |
| ATOM | 5265 | CD  | PRO | 1397 | 87.743 | 61.103              | 19.555 | 1.00 | 26.36 |
| ATOM | 5266 | CA  | PRO | 1397 | 88.134 | 60.685              | 17.218 | 1.00 | 26.48 |
| ATOM | 5267 | CB  | PRO | 1397 | 88.672 | 59.565              | 18.102 | 1.00 | 21.83 |
| ATOM | 5268 | CG  | PRO | 1397 | 88.969 | 60.251              | 19.370 | 1.00 | 22.65 |
| ATOM | 5269 | C   | PRO | 1397 | 87.080 | 60.149              | 16.261 | 1.00 | 31.18 |
| ATOM | 5270 | O   | PRO | 1397 | 85.947 | 59.901              | 16.667 | 1.00 | 31.61 |
| ATOM | 5271 | N   | GLY | 1398 | 87.435 | 60.013              | 14.988 | 1.00 | 34.68 |
| ATOM | 5272 | CA  | GLY | 1398 | 86.490 | 59.487 <sup>n</sup> | 14.023 | 1.00 | 38.08 |
| ATOM | 5273 | C   | GLY | 1398 | 86.157 | 60.474              | 12.931 | 1.00 | 41.29 |
| ATOM | 5274 | O   | GLY | 1398 | 86.563 | 61.635              | 12.975 | 1.00 | 43.61 |
| ATOM | 5275 | N   | GLU | 1399 | 85.442 | 60.001              | 11.922 | 1.00 | 42.43 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5276 | CA  | GLU | 1399 | 85.060 | 60.853 | 10.811 | 1.00 | 44.81 |
| ATOM | 5277 | CB  | GLU | 1399 | 85.423 | 60.179 | 9.485  | 1.00 | 50.25 |
| ATOM | 5278 | CG  | GLU | 1399 | 86.908 | 59.863 | 9.328  | 1.00 | 57.39 |
| ATOM | 5279 | CD  | GLU | 1399 | 87.787 | 61.093 | 9.490  | 1.00 | 63.38 |
| ATOM | 5280 | OE1 | GLU | 1399 | 87.617 | 62.057 | 8.710  | 1.00 | 64.91 |
| ATOM | 5281 | OE2 | GLU | 1399 | 88.642 | 61.097 | 10.405 | 1.00 | 66.89 |
| ATOM | 5282 | C   | GLU | 1399 | 83.564 | 61.103 | 10.876 | 1.00 | 44.39 |
| ATOM | 5283 | O   | GLU | 1399 | 82.861 | 60.497 | 11.696 | 1.00 | 45.82 |
| ATOM | 5284 | N   | TYR | 1400 | 83.081 | 62.012 | 10.038 | 1.00 | 42.99 |
| ATOM | 5285 | CA  | TYR | 1400 | 81.658 | 62.318 | 9.993  | 1.00 | 42.22 |
| ATOM | 5286 | CB  | TYR | 1400 | 81.424 | 63.815 | 9.838  | 1.00 | 38.80 |
| ATOM | 5287 | CG  | TYR | 1400 | 81.485 | 64.579 | 11.134 | 1.00 | 38.42 |
| ATOM | 5288 | CD1 | TYR | 1400 | 80.406 | 64.577 | 12.019 | 1.00 | 34.56 |
| ATOM | 5289 | CE1 | TYR | 1400 | 80.451 | 65.302 | 13.202 | 1.00 | 34.48 |
| ATOM | 5290 | CD2 | TYR | 1400 | 82.611 | 65.326 | 11.467 | 1.00 | 39.18 |
| ATOM | 5291 | CE2 | TYR | 1400 | 82.667 | 66.057 | 12.643 | 1.00 | 37.95 |
| ATOM | 5292 | CZ  | TYR | 1400 | 81.584 | 66.046 | 13.507 | 1.00 | 37.33 |
| ATOM | 5293 | OH  | TYR | 1400 | 81.637 | 66.803 | 14.656 | 1.00 | 35.83 |
| ATOM | 5294 | C   | TYR | 1400 | 81.010 | 61.592 | 8.828  | 1.00 | 43.85 |
| ATOM | 5295 | O   | TYR | 1400 | 81.693 | 61.121 | 7.915  | 1.00 | 46.67 |
| ATOM | 5296 | N   | PHE | 1401 | 79.691 | 61.485 | 8.874  | 1.00 | 42.83 |
| ATOM | 5297 | CA  | PHE | 1401 | 78.946 | 60.838 | 7.815  | 1.00 | 43.05 |
| ATOM | 5298 | CB  | PHE | 1401 | 79.094 | 59.311 | 7.881  | 1.00 | 45.25 |
| ATOM | 5299 | CG  | PHE | 1401 | 78.640 | 58.695 | 9.177  | 1.00 | 45.71 |
| ATOM | 5300 | CD1 | PHE | 1401 | 77.292 | 58.411 | 9.395  | 1.00 | 47.44 |
| ATOM | 5301 | CD2 | PHE | 1401 | 79.562 | 58.361 | 10.162 | 1.00 | 44.15 |
| ATOM | 5302 | CE1 | PHE | 1401 | 76.873 | 57.804 | 10.573 | 1.00 | 47.10 |
| ATOM | 5303 | CE2 | PHE | 1401 | 79.155 | 57.754 | 11.345 | 1.00 | 44.90 |
| ATOM | 5304 | CZ  | PHE | 1401 | 77.809 | 57.475 | 11.551 | 1.00 | 47.14 |
| ATOM | 5305 | C   | PHE | 1401 | 77.496 | 61.250 | 7.920  | 1.00 | 43.47 |
| ATOM | 5306 | O   | PHE | 1401 | 77.089 | 61.848 | 8.907  | 1.00 | 42.96 |
| ATOM | 5307 | N   | PHE | 1402 | 76.719 | 60.952 | 6.891  | 1.00 | 43.97 |
| ATOM | 5308 | CA  | PHE | 1402 | 75.322 | 61.318 | 6.899  | 1.00 | 44.22 |
| ATOM | 5309 | CB  | PHE | 1402 | 75.016 | 62.274 | 5.745  | 1.00 | 42.02 |
| ATOM | 5310 | CG  | PHE | 1402 | 75.651 | 63.622 | 5.890  | 1.00 | 38.81 |
| ATOM | 5311 | CD1 | PHE | 1402 | 77.011 | 63.797 | 5.644  | 1.00 | 39.76 |
| ATOM | 5312 | CD2 | PHE | 1402 | 74.897 | 64.716 | 6.296  | 1.00 | 35.67 |
| ATOM | 5313 | CE1 | PHE | 1402 | 77.614 | 65.049 | 5.806  | 1.00 | 38.11 |
| ATOM | 5314 | CE2 | PHE | 1402 | 75.485 | 65.969 | 6.460  | 1.00 | 35.15 |
| ATOM | 5315 | CZ  | PHE | 1402 | 76.848 | 66.136 | 6.216  | 1.00 | 36.13 |
| ATOM | 5316 | C   | PHE | 1402 | 74.438 | 60.097 | 6.739  | 1.00 | 46.31 |
| ATOM | 5317 | O   | PHE | 1402 | 74.732 | 59.177 | 6.035  | 1.00 | 46.36 |
| ATOM | 5318 | N   | SER | 1403 | 73.380 | 60.072 | 7.583  | 1.00 | 48.81 |
| ATOM | 5319 | CA  | SER | 1403 | 72.422 | 58.986 | 7.540  | 1.00 | 52.64 |
| ATOM | 5320 | CB  | SER | 1403 | 72.183 | 58.429 | 8.936  | 1.00 | 54.92 |
| ATOM | 5321 | OG  | SER | 1403 | 73.384 | 57.885 | 9.455  | 1.00 | 59.46 |
| ATOM | 5322 | C   | SER | 1403 | 71.170 | 59.648 | 6.997  | 1.00 | 55.38 |
| ATOM | 5323 | O   | SER | 1403 | 70.155 | 59.769 | 7.684  | 1.00 | 56.51 |
| ATOM | 5324 | N   | ASP | 1404 | 71.302 | 60.146 | 5.769  | 1.00 | 57.77 |
| ATOM | 5325 | CA  | ASP | 1404 | 70.240 | 60.843 | 5.048  | 1.00 | 58.06 |
| ATOM | 5326 | CB  | ASP | 1404 | 69.000 | 59.958 | 4.873  | 1.00 | 61.87 |
| ATOM | 5327 | CG  | ASP | 1404 | 68.045 | 60.501 | 3.819  | 1.00 | 67.61 |
| ATOM | 5328 | OD1 | ASP | 1404 | 68.524 | 60.956 | 2.751  | 1.00 | 65.71 |
| ATOM | 5329 | OD2 | ASP | 1404 | 66.816 | 60.469 | 4.060  | 1.00 | 72.76 |
| ATOM | 5330 | C   | ASP | 1404 | 69.877 | 62.150 | 5.735  | 1.00 | 56.48 |
| ATOM | 5331 | O   | ASP | 1404 | 68.911 | 62.228 | 6.497  | 1.00 | 55.20 |
| ATOM | 5332 | N   | GLY | 1405 | 70.685 | 63.171 | 5.470  | 1.00 | 55.34 |
| ATOM | 5333 | CA  | GLY | 1405 | 70.449 | 64.477 | 6.054  | 1.00 | 54.46 |

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FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5334 | C   | GLY | 1405 | 71.232 | 64.720 | 7.327  | 1.00 | 53.22 |
| ATOM | 5335 | O   | GLY | 1405 | 71.901 | 65.747 | 7.461  | 1.00 | 54.73 |
| ATOM | 5336 | N   | ILE | 1406 | 71.161 | 63.779 | 8.262  | 1.00 | 51.10 |
| ATOM | 5337 | CA  | ILE | 1406 | 71.872 | 63.919 | 9.528  | 1.00 | 47.34 |
| ATOM | 5338 | CB  | ILE | 1406 | 71.181 | 63.149 | 10.693 | 1.00 | 47.55 |
| ATOM | 5339 | CG2 | ILE | 1406 | 70.137 | 64.040 | 11.359 | 1.00 | 46.87 |
| ATOM | 5340 | CG1 | ILE | 1406 | 70.582 | 61.817 | 10.214 | 1.00 | 47.02 |
| ATOM | 5341 | CD1 | ILE | 1406 | 69.158 | 61.912 | 9.660  | 1.00 | 43.14 |
| ATOM | 5342 | C   | ILE | 1406 | 73.356 | 63.562 | 9.465  | 1.00 | 44.59 |
| ATOM | 5343 | O   | ILE | 1406 | 73.738 | 62.474 | 9.026  | 1.00 | 43.27 |
| ATOM | 5344 | N   | ARG | 1407 | 74.179 | 64.521 | 9.878  | 1.00 | 42.11 |
| ATOM | 5345 | CA  | ARG | 1407 | 75.628 | 64.377 | 9.910  | 1.00 | 40.01 |
| ATOM | 5346 | CB  | ARG | 1407 | 76.280 | 65.759 | 9.797  | 1.00 | 38.99 |
| ATOM | 5347 | CG  | ARG | 1407 | 77.774 | 65.750 | 9.540  | 1.00 | 34.88 |
| ATOM | 5348 | CD  | ARG | 1407 | 78.321 | 67.167 | 9.600  | 1.00 | 33.23 |
| ATOM | 5349 | NE  | ARG | 1407 | 79.698 | 67.250 | 9.123  | 1.00 | 34.81 |
| ATOM | 5350 | CZ  | ARG | 1407 | 80.671 | 67.912 | 9.745  | 1.00 | 33.80 |
| ATOM | 5351 | NH1 | ARG | 1407 | 80.430 | 68.551 | 10.883 | 1.00 | 35.60 |
| ATOM | 5352 | NH2 | ARG | 1407 | 81.881 | 67.972 | 9.207  | 1.00 | 31.88 |
| ATOM | 5353 | C   | ARG | 1407 | 75.957 | 63.749 | 11.259 | 1.00 | 39.81 |
| ATOM | 5354 | O   | ARG | 1407 | 75.848 | 64.399 | 12.299 | 1.00 | 40.00 |
| ATOM | 5355 | N   | LEU | 1408 | 76.299 | 62.469 | 11.240 | 1.00 | 39.11 |
| ATOM | 5356 | CA  | LEU | 1408 | 76.610 | 61.734 | 12.451 | 1.00 | 38.94 |
| ATOM | 5357 | CB  | LEU | 1408 | 75.765 | 60.464 | 12.489 | 1.00 | 35.80 |
| ATOM | 5358 | CG  | LEU | 1408 | 74.271 | 60.639 | 12.265 | 1.00 | 33.00 |
| ATOM | 5359 | CD1 | LEU | 1408 | 73.658 | 59.302 | 12.000 | 1.00 | 35.13 |
| ATOM | 5360 | CD2 | LEU | 1408 | 73.637 | 61.293 | 13.466 | 1.00 | 33.45 |
| ATOM | 5361 | C   | LEU | 1408 | 78.077 | 61.349 | 12.582 | 1.00 | 39.97 |
| ATOM | 5362 | O   | LEU | 1408 | 78.846 | 61.421 | 11.621 | 1.00 | 41.20 |
| ATOM | 5363 | N   | LYS | 1409 | 78.444 | 60.922 | 13.784 | 1.00 | 39.40 |
| ATOM | 5364 | CA  | LYS | 1409 | 79.793 | 60.475 | 14.088 | 1.00 | 37.55 |
| ATOM | 5365 | CB  | LYS | 1409 | 80.574 | 61.559 | 14.812 | 1.00 | 34.49 |
| ATOM | 5366 | CG  | LYS | 1409 | 82.070 | 61.410 | 14.684 | 1.00 | 31.73 |
| ATOM | 5367 | CD  | LYS | 1409 | 82.748 | 62.681 | 15.122 | 1.00 | 31.14 |
| ATOM | 5368 | CE  | LYS | 1409 | 84.117 | 62.821 | 14.504 | 1.00 | 30.59 |
| ATOM | 5369 | NZ  | LYS | 1409 | 84.738 | 64.118 | 14.889 | 1.00 | 30.87 |
| ATOM | 5370 | C   | LYS | 1409 | 79.616 | 59.261 | 14.990 | 1.00 | 38.36 |
| ATOM | 5371 | O   | LYS | 1409 | 78.648 | 59.181 | 15.760 | 1.00 | 38.95 |
| ATOM | 5372 | N   | LYS | 1410 | 80.538 | 58.314 | 14.878 | 1.00 | 37.52 |
| ATOM | 5373 | CA  | LYS | 1410 | 80.481 | 57.083 | 15.654 | 1.00 | 37.57 |
| ATOM | 5374 | CB  | LYS | 1410 | 81.473 | 56.045 | 15.106 | 1.00 | 39.72 |
| ATOM | 5375 | CG  | LYS | 1410 | 81.424 | 55.848 | 13.586 | 1.00 | 47.39 |
| ATOM | 5376 | CD  | LYS | 1410 | 82.257 | 56.898 | 12.828 | 1.00 | 54.46 |
| ATOM | 5377 | CE  | LYS | 1410 | 83.704 | 56.437 | 12.552 | 1.00 | 57.97 |
| ATOM | 5378 | NZ  | LYS | 1410 | 84.528 | 56.135 | 13.772 | 1.00 | 58.51 |
| ATOM | 5379 | C   | LYS | 1410 | 80.737 | 57.292 | 17.144 | 1.00 | 36.58 |
| ATOM | 5380 | O   | LYS | 1410 | 81.503 | 58.169 | 17.548 | 1.00 | 36.90 |
| ATOM | 5381 | N   | TYR | 1411 | 80.045 | 56.504 | 17.956 | 1.00 | 33.81 |
| ATOM | 5382 | CA  | TYR | 1411 | 80.196 | 56.538 | 19.398 | 1.00 | 29.59 |
| ATOM | 5383 | CB  | TYR | 1411 | 79.308 | 57.606 | 20.036 | 1.00 | 28.89 |
| ATOM | 5384 | CG  | TYR | 1411 | 79.468 | 57.638 | 21.536 | 1.00 | 29.67 |
| ATOM | 5385 | CD1 | TYR | 1411 | 80.735 | 57.684 | 22.113 | 1.00 | 27.56 |
| ATOM | 5386 | CE1 | TYR | 1411 | 80.900 | 57.654 | 23.484 | 1.00 | 32.21 |
| ATOM | 5387 | CD2 | TYR | 1411 | 78.363 | 57.575 | 22.380 | 1.00 | 32.44 |
| ATOM | 5388 | CE2 | TYR | 1411 | 78.515 | 57.547 | 23.767 | 1.00 | 35.34 |
| ATOM | 5389 | CZ  | TYR | 1411 | 79.792 | 57.588 | 24.313 | 1.00 | 35.21 |
| ATOM | 5390 | OH  | TYR | 1411 | 79.975 | 57.562 | 25.683 | 1.00 | 32.62 |
| ATOM | 5391 | C   | TYR | 1411 | 79.794 | 55.156 | 19.890 | 1.00 | 28.28 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5392 | O   | TYR | 1411 | 78.666 | 54.717 | 19.658 | 1.00 | 29.51 |
| ATOM | 5393 | N   | ARG | 1412 | 80.705 | 54.482 | 20.583 | 1.00 | 25.07 |
| ATOM | 5394 | CA  | ARG | 1412 | 80.442 | 53.131 | 21.067 | 1.00 | 22.53 |
| ATOM | 5395 | CB  | ARG | 1412 | 81.072 | 52.122 | 20.104 | 1.00 | 22.14 |
| ATOM | 5396 | CG  | ARG | 1412 | 82.573 | 52.254 | 20.020 | 1.00 | 22.85 |
| ATOM | 5397 | CD  | ARG | 1412 | 83.202 | 51.252 | 19.099 | 1.00 | 21.78 |
| ATOM | 5398 | NE  | ARG | 1412 | 84.655 | 51.364 | 19.163 | 1.00 | 24.40 |
| ATOM | 5399 | CZ  | ARG | 1412 | 85.496 | 50.726 | 18.355 | 1.00 | 28.25 |
| ATOM | 5400 | NH1 | ARG | 1412 | 85.037 | 49.921 | 17.410 | 1.00 | 29.33 |
| ATOM | 5401 | NH2 | ARG | 1412 | 86.803 | 50.887 | 18.501 | 1.00 | 31.56 |
| ATOM | 5402 | C   | ARG | 1412 | 80.980 | 52.865 | 22.469 | 1.00 | 20.00 |
| ATOM | 5403 | O   | ARG | 1412 | 81.990 | 53.437 | 22.881 | 1.00 | 19.85 |
| ATOM | 5404 | N   | GLY | 1413 | 80.316 | 51.966 | 23.183 | 1.00 | 18.06 |
| ATOM | 5405 | CA  | GLY | 1413 | 80.765 | 51.618 | 24.512 | 1.00 | 18.17 |
| ATOM | 5406 | C   | GLY | 1413 | 82.049 | 50.841 | 24.373 | 1.00 | 19.69 |
| ATOM | 5407 | O   | GLY | 1413 | 82.237 | 50.126 | 23.384 | 1.00 | 19.71 |
| ATOM | 5408 | N   | MET | 1414 | 82.944 | 50.988 | 25.342 | 1.00 | 20.34 |
| ATOM | 5409 | CA  | MET | 1414 | 84.221 | 50.282 | 25.309 | 1.00 | 22.12 |
| ATOM | 5410 | CB  | MET | 1414 | 85.180 | 50.857 | 26.356 | 1.00 | 22.03 |
| ATOM | 5411 | CG  | MET | 1414 | 85.671 | 52.265 | 26.041 | 1.00 | 23.32 |
| ATOM | 5412 | SD  | MET | 1414 | 86.555 | 52.417 | 24.466 | 1.00 | 26.75 |
| ATOM | 5413 | CE  | MET | 1414 | 85.214 | 52.711 | 23.391 | 1.00 | 28.28 |
| ATOM | 5414 | C   | MET | 1414 | 84.040 | 48.781 | 25.504 | 1.00 | 22.54 |
| ATOM | 5415 | O   | MET | 1414 | 84.896 | 47.981 | 25.112 | 1.00 | 23.42 |
| ATOM | 5416 | N   | GLY | 1415 | 82.907 | 48.405 | 26.086 | 1.00 | 22.77 |
| ATOM | 5417 | CA  | GLY | 1415 | 82.626 | 47.006 | 26.313 | 1.00 | 22.65 |
| ATOM | 5418 | C   | GLY | 1415 | 81.802 | 46.428 | 25.190 | 1.00 | 23.70 |
| ATOM | 5419 | O   | GLY | 1415 | 81.146 | 45.412 | 25.378 | 1.00 | 24.44 |
| ATOM | 5420 | N   | SER | 1416 | 81.783 | 47.091 | 24.039 | 1.00 | 25.46 |
| ATOM | 5421 | CA  | SER | 1416 | 81.025 | 46.578 | 22.911 | 1.00 | 28.36 |
| ATOM | 5422 | CB  | SER | 1416 | 80.623 | 47.703 | 21.945 | 1.00 | 26.46 |
| ATOM | 5423 | OG  | SER | 1416 | 81.743 | 48.329 | 21.341 | 1.00 | 25.07 |
| ATOM | 5424 | C   | SER | 1416 | 81.858 | 45.522 | 22.194 | 1.00 | 32.07 |
| ATOM | 5425 | O   | SER | 1416 | 83.089 | 45.526 | 22.278 | 1.00 | 32.48 |
| ATOM | 5426 | N   | LEU | 1417 | 81.175 | 44.625 | 21.490 | 1.00 | 35.05 |
| ATOM | 5427 | CA  | LEU | 1417 | 81.815 | 43.551 | 20.746 | 1.00 | 37.86 |
| ATOM | 5428 | CB  | LEU | 1417 | 80.744 | 42.758 | 19.989 | 1.00 | 37.24 |
| ATOM | 5429 | CG  | LEU | 1417 | 80.467 | 41.322 | 20.443 | 1.00 | 36.80 |
| ATOM | 5430 | CD1 | LEU | 1417 | 81.602 | 40.422 | 19.990 | 1.00 | 41.48 |
| ATOM | 5431 | CD2 | LEU | 1417 | 80.305 | 41.258 | 21.948 | 1.00 | 32.76 |
| ATOM | 5432 | C   | LEU | 1417 | 82.909 | 44.029 | 19.777 | 1.00 | 41.62 |
| ATOM | 5433 | O   | LEU | 1417 | 83.996 | 43.447 | 19.726 | 1.00 | 42.91 |
| ATOM | 5434 | N   | ASP | 1418 | 82.625 | 45.096 | 19.029 | 1.00 | 43.98 |
| ATOM | 5435 | CA  | ASP | 1418 | 83.582 | 45.628 | 18.056 | 1.00 | 44.77 |
| ATOM | 5436 | CB  | ASP | 1418 | 82.852 | 46.360 | 16.916 | 1.00 | 45.89 |
| ATOM | 5437 | CG  | ASP | 1418 | 82.267 | 47.696 | 17.345 | 1.00 | 49.84 |
| ATOM | 5438 | OD1 | ASP | 1418 | 81.466 | 47.728 | 18.304 | 1.00 | 54.75 |
| ATOM | 5439 | OD2 | ASP | 1418 | 82.600 | 48.718 | 16.706 | 1.00 | 49.55 |
| ATOM | 5440 | C   | ASP | 1418 | 84.658 | 46.521 | 18.672 | 1.00 | 44.00 |
| ATOM | 5441 | O   | ASP | 1418 | 85.700 | 46.754 | 18.067 | 1.00 | 45.96 |
| ATOM | 5442 | N   | ALA | 1419 | 84.383 | 47.068 | 19.848 | 1.00 | 42.92 |
| ATOM | 5443 | CA  | ALA | 1419 | 85.363 | 47.908 | 20.511 | 1.00 | 41.90 |
| ATOM | 5444 | CB  | ALA | 1419 | 84.712 | 48.728 | 21.612 | 1.00 | 39.79 |
| ATOM | 5445 | C   | ALA | 1419 | 86.398 | 46.970 | 21.100 | 1.00 | 42.91 |
| ATOM | 5446 | O   | ALA | 1419 | 87.598 | 47.217 | 20.994 | 1.00 | 43.77 |
| ATOM | 5447 | N   | MET | 1420 | 85.919 | 45.878 | 21.692 | 1.00 | 44.17 |
| ATOM | 5448 | CA  | MET | 1420 | 86.783 | 44.882 | 22.324 | 1.00 | 46.58 |
| ATCM | 5449 | CB  | MET | 1420 | 85.960 | 43.956 | 23.228 | 1.00 | 44.85 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5450 | CG  | MET | 1420 | 85.222 | 44.663 | 24.359 | 1.00 | 40.59 |
| ATOM | 5451 | SD  | MET | 1420 | 84.557 | 43.506 | 25.583 | 1.00 | 37.46 |
| ATOM | 5452 | CE  | MET | 1420 | 83.211 | 42.736 | 24.659 | 1.00 | 35.09 |
| ATOM | 5453 | C   | MET | 1420 | 87.615 | 44.049 | 21.340 | 1.00 | 48.15 |
| ATOM | 5454 | O   | MET | 1420 | 87.079 | 43.674 | 20.273 | 1.00 | 49.93 |
| ATOM | 5455 | CB  | ILE | 1437 | 81.342 | 33.951 | 22.925 | 1.00 | 66.55 |
| ATOM | 5456 | CG2 | ILE | 1437 | 81.311 | 33.579 | 21.441 | 1.00 | 68.42 |
| ATOM | 5457 | CG1 | ILE | 1437 | 80.618 | 32.891 | 23.774 | 1.00 | 66.87 |
| ATOM | 5458 | CD1 | ILE | 1437 | 80.344 | 33.296 | 25.209 | 1.00 | 65.86 |
| ATOM | 5459 | C   | ILE | 1437 | 82.900 | 35.253 | 24.433 | 1.00 | 60.65 |
| ATOM | 5460 | O   | ILE | 1437 | 83.257 | 34.991 | 25.582 | 1.00 | 60.18 |
| ATOM | 5461 | N   | ILE | 1437 | 83.398 | 32.887 | 23.943 | 1.00 | 64.00 |
| ATOM | 5462 | CA  | ILE | 1437 | 82.815 | 34.144 | 23.394 | 1.00 | 63.11 |
| ATOM | 5463 | N   | LYS | 1438 | 82.590 | 36.480 | 24.022 | 1.00 | 58.06 |
| ATOM | 5464 | CA  | LYS | 1438 | 82.649 | 37.632 | 24.916 | 1.00 | 54.30 |
| ATOM | 5465 | CB  | LYS | 1438 | 83.479 | 38.752 | 24.283 | 1.00 | 57.05 |
| ATOM | 5466 | CG  | LYS | 1438 | 84.954 | 36.440 | 24.118 | 1.00 | 61.76 |
| ATOM | 5467 | CD  | LYS | 1438 | 85.719 | 39.680 | 23.684 | 1.00 | 66.01 |
| ATOM | 5468 | CE  | LYS | 1438 | 87.222 | 39.446 | 23.713 | 1.00 | 70.05 |
| ATOM | 5469 | NZ  | LYS | 1438 | 87.994 | 40.707 | 23.490 | 1.00 | 72.96 |
| ATOM | 5470 | C   | LYS | 1438 | 81.264 | 38.170 | 25.269 | 1.00 | 50.75 |
| ATOM | 5471 | O   | LYS | 1438 | 80.359 | 38.186 | 24.437 | 1.00 | 51.21 |
| ATOM | 5472 | N   | VAL | 1439 | 81.109 | 38.618 | 26.508 | 1.00 | 47.03 |
| ATOM | 5473 | CA  | VAL | 1439 | 79.841 | 39.171 | 26.969 | 1.00 | 42.02 |
| ATOM | 5474 | CB  | VAL | 1439 | 79.561 | 38.776 | 28.441 | 1.00 | 39.60 |
| ATOM | 5475 | CG1 | VAL | 1439 | 78.227 | 39.331 | 28.893 | 1.00 | 37.77 |
| ATOM | 5476 | CG2 | VAL | 1439 | 79.573 | 37.261 | 28.589 | 1.00 | 37.89 |
| ATOM | 5477 | C   | VAL | 1439 | 79.903 | 40.694 | 26.830 | 1.00 | 39.68 |
| ATOM | 5478 | O   | VAL | 1439 | 80.562 | 41.372 | 27.623 | 1.00 | 39.64 |
| ATOM | 5479 | N   | ALA | 1440 | 79.266 | 41.214 | 25.782 | 1.00 | 36.52 |
| ATOM | 5480 | CA  | ALA | 1440 | 79.244 | 42.651 | 25.514 | 1.00 | 33.16 |
| ATOM | 5481 | CB  | ALA | 1440 | 78.640 | 42.931 | 24.151 | 1.00 | 33.07 |
| ATOM | 5482 | C   | ALA | 1440 | 78.487 | 43.425 | 26.578 | 1.00 | 31.48 |
| ATOM | 5483 | O   | ALA | 1440 | 77.377 | 43.055 | 26.964 | 1.00 | 31.26 |
| ATOM | 5484 | N   | GLN | 1441 | 79.092 | 44.517 | 27.031 | 1.00 | 30.45 |
| ATOM | 5485 | CA  | GLN | 1441 | 78.497 | 45.369 | 28.049 | 1.00 | 27.44 |
| ATOM | 5486 | CB  | GLN | 1441 | 79.453 | 45.525 | 29.225 | 1.00 | 23.78 |
| ATOM | 5487 | CG  | GLN | 1441 | 79.765 | 44.207 | 29.902 | 1.00 | 22.17 |
| ATOM | 5488 | CD  | GLN | 1441 | 80.382 | 44.395 | 31.258 | 1.00 | 23.37 |
| ATOM | 5489 | OE1 | GLN | 1441 | 79.840 | 45.109 | 32.100 | 1.00 | 22.22 |
| ATOM | 5490 | NE2 | GLN | 1441 | 81.515 | 43.750 | 31.489 | 1.00 | 25.42 |
| ATOM | 5491 | C   | GLN | 1441 | 78.086 | 46.733 | 27.501 | 1.00 | 28.00 |
| ATOM | 5492 | O   | GLN | 1441 | 77.548 | 47.565 | 28.230 | 1.00 | 28.70 |
| ATOM | 5493 | N   | GLY | 1442 | 78.273 | 46.929 | 26.200 | 1.00 | 28.38 |
| ATOM | 5494 | CA  | GLY | 1442 | 77.905 | 48.184 | 25.576 | 1.00 | 27.33 |
| ATOM | 5495 | C   | GLY | 1442 | 77.463 | 47.982 | 24.138 | 1.00 | 27.30 |
| ATOM | 5496 | O   | GLY | 1442 | 77.656 | 46.902 | 23.564 | 1.00 | 27.61 |
| ATOM | 5497 | N   | VAL | 1443 | 76.833 | 49.005 | 23.572 | 1.00 | 26.10 |
| ATOM | 5498 | CA  | VAL | 1443 | 76.376 | 48.970 | 22.187 | 1.00 | 23.86 |
| ATOM | 5499 | CB  | VAL | 1443 | 74.867 | 49.329 | 22.057 | 1.00 | 21.54 |
| ATOM | 5500 | CG1 | VAL | 1443 | 74.027 | 48.384 | 22.884 | 1.00 | 16.72 |
| ATOM | 5501 | CG2 | VAL | 1443 | 74.618 | 50.775 | 22.470 | 1.00 | 21.56 |
| ATOM | 5502 | C   | VAL | 1443 | 77.202 | 49.988 | 21.406 | 1.00 | 23.54 |
| ATOM | 5503 | O   | VAL | 1443 | 77.823 | 50.877 | 21.995 | 1.00 | 23.22 |
| ATOM | 5504 | N   | SER | 1444 | 77.234 | 49.841 | 20.088 | 1.00 | 24.09 |
| ATOM | 5505 | CA  | SER | 1444 | 77.980 | 50.765 | 19.248 | 1.00 | 23.73 |
| ATOM | 5506 | CB  | SER | 1444 | 78.953 | 49.995 | 18.359 | 1.00 | 24.52 |
| ATCM | 5507 | OG  | SER | 1444 | 79.897 | 50.872 | 17.774 | 1.00 | 30.92 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5508 | C   | SER | 1444 | 76.972 | 51.502 | 18.392 | 1.00 | 24.25 |
| ATOM | 5509 | O   | SER | 1444 | 76.180 | 50.874 | 17.689 | 1.00 | 25.44 |
| ATOM | 5510 | N   | GLY | 1445 | 76.973 | 52.825 | 18.454 | 1.00 | 24.61 |
| ATOM | 5511 | CA  | GLY | 1445 | 76.017 | 53.576 | 17.662 | 1.00 | 26.65 |
| ATOM | 5512 | C   | GLY | 1445 | 76.569 | 54.849 | 17.063 | 1.00 | 28.09 |
| ATOM | 5513 | O   | GLY | 1445 | 77.767 | 54.951 | 16.794 | 1.00 | 29.89 |
| ATOM | 5514 | N   | ALA | 1446 | 75.695 | 55.822 | 16.841 | 1.00 | 27.70 |
| ATOM | 5515 | CA  | ALA | 1446 | 76.112 | 57.090 | 16.272 | 1.00 | 28.08 |
| ATOM | 5516 | CB  | ALA | 1446 | 75.848 | 57.105 | 14.782 | 1.00 | 25.75 |
| ATOM | 5517 | C   | ALA | 1446 | 75.364 | 58.220 | 16.947 | 1.00 | 29.63 |
| ATOM | 5518 | O   | ALA | 1446 | 74.307 | 58.004 | 17.543 | 1.00 | 29.07 |
| ATOM | 5519 | N   | VAL | 1447 | 75.935 | 59.416 | 16.879 | 1.00 | 31.82 |
| ATOM | 5520 | CA  | VAL | 1447 | 75.325 | 60.612 | 17.454 | 1.00 | 35.50 |
| ATOM | 5521 | CB  | VAL | 1447 | 75.954 | 60.996 | 18.819 | 1.00 | 38.59 |
| ATOM | 5522 | CG1 | VAL | 1447 | 75.443 | 60.074 | 19.917 | 1.00 | 41.19 |
| ATOM | 5523 | CG2 | VAL | 1447 | 77.464 | 60.914 | 18.744 | 1.00 | 41.83 |
| ATOM | 5524 | C   | VAL | 1447 | 75.471 | 61.767 | 16.460 | 1.00 | 36.50 |
| ATOM | 5525 | O   | VAL | 1447 | 76.389 | 61.781 | 15.633 | 1.00 | 36.46 |
| ATOM | 5526 | N   | GLN | 1448 | 74.543 | 62.715 | 16.527 | 1.00 | 37.04 |
| ATOM | 5527 | CA  | GLN | 1448 | 74.538 | 63.863 | 15.632 | 1.00 | 37.13 |
| ATOM | 5528 | CB  | GLN | 1448 | 73.145 | 64.492 | 15.624 | 1.00 | 40.18 |
| ATOM | 5529 | CG  | GLN | 1448 | 72.945 | 65.593 | 14.589 | 1.00 | 42.82 |
| ATOM | 5530 | CD  | GLN | 1448 | 71.498 | 66.047 | 14.492 | 1.00 | 42.85 |
| ATOM | 5531 | OE1 | GLN | 1448 | 70.612 | 65.492 | 15.146 | 1.00 | 41.67 |
| ATOM | 5532 | NE2 | GLN | 1448 | 71.251 | 67.054 | 13.666 | 1.00 | 43.75 |
| ATOM | 5533 | C   | GLN | 1448 | 75.603 | 64.919 | 15.941 | 1.00 | 36.41 |
| ATOM | 5534 | O   | GLN | 1448 | 75.812 | 65.298 | 17.096 | 1.00 | 37.30 |
| ATOM | 5535 | N   | ASP | 1449 | 76.263 | 65.383 | 14.885 | 1.00 | 35.19 |
| ATOM | 5536 | CA  | ASP | 1449 | 77.311 | 66.399 | 14.941 | 1.00 | 34.49 |
| ATOM | 5537 | CB  | ASP | 1449 | 77.536 | 66.948 | 13.524 | 1.00 | 33.54 |
| ATOM | 5538 | CG  | ASP | 1449 | 78.452 | 68.160 | 13.483 | 1.00 | 34.61 |
| ATOM | 5539 | OD1 | ASP | 1449 | 79.444 | 68.210 | 14.242 | 1.00 | 34.88 |
| ATOM | 5540 | OD2 | ASP | 1449 | 78.183 | 69.063 | 12.663 | 1.00 | 35.64 |
| ATOM | 5541 | C   | ASP | 1449 | 76.961 | 67.537 | 15.896 | 1.00 | 33.86 |
| ATOM | 5542 | O   | ASP | 1449 | 76.038 | 68.301 | 15.642 | 1.00 | 35.06 |
| ATOM | 5543 | N   | LYS | 1450 | 77.714 | 67.647 | 16.986 | 1.00 | 33.79 |
| ATOM | 5544 | CA  | LYS | 1450 | 77.487 | 68.696 | 17.977 | 1.00 | 34.79 |
| ATOM | 5545 | CB  | LYS | 1450 | 77.726 | 68.163 | 19.393 | 1.00 | 38.05 |
| ATOM | 5546 | CG  | LYS | 1450 | 76.750 | 67.084 | 19.820 | 1.00 | 47.10 |
| ATOM | 5547 | CD  | LYS | 1450 | 77.088 | 66.552 | 21.200 | 1.00 | 52.04 |
| ATOM | 5548 | CE  | LYS | 1450 | 76.150 | 65.422 | 21.602 | 1.00 | 57.04 |
| ATOM | 5549 | NZ  | LYS | 1450 | 76.264 | 64.232 | 20.705 | 1.00 | 59.52 |
| ATOM | 5550 | C   | LYS | 1450 | 78.356 | 69.931 | 17.754 | 1.00 | 33.28 |
| ATOM | 5551 | O   | LYS | 1450 | 78.324 | 70.864 | 18.555 | 1.00 | 34.18 |
| ATOM | 5552 | N   | GLY | 1451 | 79.148 | 69.934 | 16.687 | 1.00 | 32.00 |
| ATOM | 5553 | CA  | GLY | 1451 | 80.005 | 71.074 | 16.413 | 1.00 | 29.42 |
| ATOM | 5554 | C   | GLY | 1451 | 81.354 | 70.937 | 17.086 | 1.00 | 28.07 |
| ATOM | 5555 | O   | GLY | 1451 | 81.808 | 69.818 | 17.335 | 1.00 | 26.57 |
| ATOM | 5556 | N   | SER | 1452 | 81.971 | 72.066 | 17.426 | 1.00 | 27.12 |
| ATOM | 5557 | CA  | SER | 1452 | 83.290 | 72.062 | 18.058 | 1.00 | 26.69 |
| ATOM | 5558 | CB  | SER | 1452 | 84.206 | 73.084 | 17.364 | 1.00 | 30.79 |
| ATOM | 5559 | OG  | SER | 1452 | 85.474 | 73.215 | 18.000 | 1.00 | 30.53 |
| ATOM | 5560 | C   | SER | 1452 | 83.285 | 72.312 | 19.560 | 1.00 | 25.17 |
| ATOM | 5561 | O   | SER | 1452 | 82.528 | 73.154 | 20.057 | 1.00 | 25.27 |
| ATOM | 5562 | N   | ILE | 1453 | 84.186 | 71.615 | 20.259 | 1.00 | 23.64 |
| ATOM | 5563 | CA  | ILE | 1453 | 84.360 | 71.724 | 21.712 | 1.00 | 21.74 |
| ATOM | 5564 | CB  | ILE | 1453 | 85.588 | 70.911 | 22.193 | 1.00 | 18.90 |
| ATOM | 5565 | CG2 | ILE | 1453 | 86.084 | 71.414 | 23.541 | 1.00 | 15.69 |



FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5566 | CG1 | ILE | 1453 | 85.247 | 69.420 | 22.276 | 1.00 | 18.69 |
| ATOM | 5567 | CD1 | ILE | 1453 | 84.246 | 69.068 | 23.344 | 1.00 | 16.28 |
| ATOM | 5568 | C   | ILE | 1453 | 84.571 | 73.172 | 22.119 | 1.00 | 23.00 |
| ATOM | 5569 | O   | ILE | 1453 | 84.144 | 73.598 | 23.192 | 1.00 | 23.69 |
| ATOM | 5570 | N   | HIS | 1454 | 85.195 | 73.931 | 21.228 | 1.00 | 25.62 |
| ATOM | 5571 | CA  | HIS | 1454 | 85.494 | 75.331 | 21.472 | 1.00 | 26.80 |
| ATOM | 5572 | CB  | HIS | 1454 | 86.497 | 75.828 | 20.437 | 1.00 | 26.77 |
| ATOM | 5573 | CG  | HIS | 1454 | 87.850 | 75.202 | 20.581 | 1.00 | 29.51 |
| ATOM | 5574 | CD2 | HIS | 1454 | 88.430 | 74.172 | 19.927 | 1.00 | 28.95 |
| ATOM | 5575 | ND1 | HIS | 1454 | 88.757 | 75.608 | 21.538 | 1.00 | 33.65 |
| ATOM | 5576 | CE1 | HIS | 1454 | 89.836 | 74.848 | 21.470 | 1.00 | 33.07 |
| ATOM | 5577 | NE2 | HIS | 1454 | 89.663 | 73.971 | 20.498 | 1.00 | 31.26 |
| ATOM | 5578 | C   | HIS | 1454 | 84.281 | 76.251 | 21.580 | 1.00 | 27.40 |
| ATOM | 5579 | O   | HIS | 1454 | 84.418 | 77.414 | 21.963 | 1.00 | 25.97 |
| ATOM | 5580 | N   | LYS | 1455 | 83.103 | 75.725 | 21.259 | 1.00 | 27.47 |
| ATOM | 5581 | CA  | LYS | 1455 | 81.864 | 76.488 | 21.360 | 1.00 | 30.12 |
| ATOM | 5582 | CB  | LYS | 1455 | 81.153 | 76.575 | 20.012 | 1.00 | 35.92 |
| ATOM | 5583 | CG  | LYS | 1455 | 81.922 | 77.286 | 18.917 | 1.00 | 45.61 |
| ATOM | 5584 | CD  | LYS | 1455 | 81.370 | 76.898 | 17.543 | 1.00 | 57.31 |
| ATOM | 5585 | CE  | LYS | 1455 | 81.386 | 75.368 | 17.347 | 1.00 | 61.81 |
| ATOM | 5586 | NZ  | LYS | 1455 | 80.920 | 74.895 | 16.006 | 1.00 | 60.26 |
| ATOM | 5587 | C   | LYS | 1455 | 80.950 | 75.771 | 22.344 | 1.00 | 28.06 |
| ATOM | 5588 | O   | LYS | 1455 | 80.318 | 76.399 | 23.195 | 1.00 | 30.49 |
| ATOM | 5589 | N   | PHE | 1456 | 80.915 | 74.446 | 22.242 | 1.00 | 24.81 |
| ATOM | 5590 | CA  | PHE | 1456 | 80.071 | 73.625 | 23.096 | 1.00 | 20.59 |
| ATOM | 5591 | CB  | PHE | 1456 | 80.105 | 72.165 | 22.636 | 1.00 | 21.85 |
| ATOM | 5592 | CG  | PHE | 1456 | 79.036 | 71.314 | 23.258 | 1.00 | 23.75 |
| ATOM | 5593 | CD1 | PHE | 1456 | 77.723 | 71.383 | 22.797 | 1.00 | 20.86 |
| ATOM | 5594 | CD2 | PHE | 1456 | 79.328 | 70.479 | 24.335 | 1.00 | 27.64 |
| ATOM | 5595 | CE1 | PHE | 1456 | 76.714 | 70.636 | 23.404 | 1.00 | 21.49 |
| ATOM | 5596 | CE2 | PHE | 1456 | 78.325 | 69.729 | 24.945 | 1.00 | 22.84 |
| ATOM | 5597 | CZ  | PHE | 1456 | 77.015 | 69.810 | 24.480 | 1.00 | 20.55 |
| ATOM | 5598 | C   | PHE | 1456 | 80.411 | 73.729 | 24.579 | 1.00 | 17.53 |
| ATOM | 5599 | O   | PHE | 1456 | 79.529 | 73.929 | 25.403 | 1.00 | 15.84 |
| ATOM | 5600 | N   | VAL | 1457 | 81.682 | 73.586 | 24.928 | 1.00 | 17.91 |
| ATOM | 5601 | CA  | VAL | 1457 | 82.073 | 73.685 | 26.329 | 1.00 | 19.08 |
| ATOM | 5602 | CB  | VAL | 1457 | 83.571 | 73.399 | 26.536 | 1.00 | 15.14 |
| ATOM | 5603 | CG1 | VAL | 1457 | 83.994 | 73.760 | 27.953 | 1.00 | 13.44 |
| ATOM | 5604 | CG2 | VAL | 1457 | 83.833 | 71.932 | 26.304 | 1.00 | 16.34 |
| ATOM | 5605 | C   | VAL | 1457 | 81.681 | 75.051 | 26.904 | 1.00 | 22.53 |
| ATOM | 5606 | O   | VAL | 1457 | 81.080 | 75.131 | 27.983 | 1.00 | 22.20 |
| ATOM | 5607 | N   | PRO | 1458 | 82.013 | 76.145 | 26.191 | 1.00 | 24.20 |
| ATOM | 5608 | CD  | PRO | 1458 | 82.911 | 76.261 | 25.027 | 1.00 | 24.44 |
| ATOM | 5609 | CA  | PRO | 1458 | 81.651 | 77.475 | 26.695 | 1.00 | 25.28 |
| ATOM | 5610 | CB  | PRO | 1458 | 82.122 | 78.392 | 25.573 | 1.00 | 27.34 |
| ATOM | 5611 | CG  | PRO | 1458 | 83.363 | 77.702 | 25.107 | 1.00 | 25.79 |
| ATOM | 5612 | C   | PRO | 1458 | 80.147 | 77.576 | 26.939 | 1.00 | 24.20 |
| ATOM | 5613 | O   | PRO | 1458 | 79.693 | 78.307 | 27.823 | 1.00 | 25.91 |
| ATOM | 5614 | N   | TYR | 1459 | 79.373 | 76.849 | 26.147 | 1.00 | 22.70 |
| ATOM | 5615 | CA  | TYR | 1459 | 77.934 | 76.832 | 26.337 | 1.00 | 22.83 |
| ATOM | 5616 | CB  | TYR | 1459 | 77.255 | 76.104 | 25.177 | 1.00 | 21.77 |
| ATOM | 5617 | CG  | TYR | 1459 | 75.901 | 75.539 | 25.531 | 1.00 | 26.38 |
| ATOM | 5618 | CD1 | TYR | 1459 | 74.833 | 76.374 | 25.869 | 1.00 | 29.53 |
| ATOM | 5619 | CE1 | TYR | 1459 | 73.595 | 75.845 | 26.230 | 1.00 | 30.45 |
| ATOM | 5620 | CD2 | TYR | 1459 | 75.693 | 74.160 | 25.559 | 1.00 | 28.56 |
| ATOM | 5621 | CE2 | TYR | 1459 | 74.462 | 73.619 | 25.917 | 1.00 | 26.79 |
| ATOM | 5622 | CZ  | TYR | 1459 | 73.419 | 74.463 | 26.250 | 1.00 | 28.78 |
| ATOM | 5623 | OH  | TYR | 1459 | 72.209 | 73.912 | 26.604 | 1.00 | 26.01 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5624 | C   | TYR | 1459 | 77.635 | 76.123 | 27.669 | 1.00 | 22.79 |
| ATOM | 5625 | O   | TYR | 1459 | 76.879 | 76.634 | 28.497 | 1.00 | 22.57 |
| ATOM | 5626 | N   | LEU | 1460 | 78.261 | 74.966 | 27.883 | 1.00 | 22.45 |
| ATOM | 5627 | CA  | LEU | 1460 | 78.062 | 74.188 | 29.105 | 1.00 | 20.94 |
| ATOM | 5628 | CB  | LEU | 1460 | 78.909 | 72.908 | 29.091 | 1.00 | 18.74 |
| ATOM | 5629 | CG  | LEU | 1460 | 78.564 | 71.821 | 28.062 | 1.00 | 15.82 |
| ATOM | 5630 | CD1 | LEU | 1460 | 79.566 | 70.675 | 28.136 | 1.00 | 11.15 |
| ATOM | 5631 | CD2 | LEU | 1460 | 77.157 | 71.307 | 28.295 | 1.00 | 12.28 |
| ATOM | 5632 | C   | LEU | 1460 | 78.376 | 75.016 | 30.341 | 1.00 | 20.69 |
| ATOM | 5633 | O   | LEU | 1460 | 77.619 | 75.015 | 31.309 | 1.00 | 22.07 |
| ATOM | 5634 | N   | ILE | 1461 | 79.486 | 75.737 | 30.301 | 1.00 | 21.57 |
| ATOM | 5635 | CA  | ILE | 1461 | 79.880 | 76.583 | 31.423 | 1.00 | 22.27 |
| ATOM | 5636 | CB  | ILE | 1461 | 81.223 | 77.296 | 31.134 | 1.00 | 18.97 |
| ATOM | 5637 | CG2 | ILE | 1461 | 81.550 | 78.264 | 32.239 | 1.00 | 19.35 |
| ATOM | 5638 | CG1 | ILE | 1461 | 82.346 | 76.269 | 30.990 | 1.00 | 15.84 |
| ATOM | 5639 | CD1 | ILE | 1461 | 83.661 | 76.851 | 30.523 | 1.00 | 15.19 |
| ATOM | 5640 | C   | ILE | 1461 | 78.785 | 77.623 | 31.683 | 1.00 | 22.73 |
| ATOM | 5641 | O   | ILE | 1461 | 78.374 | 77.849 | 32.823 | 1.00 | 24.12 |
| ATOM | 5642 | N   | ALA | 1462 | 78.286 | 78.233 | 30.618 | 1.00 | 22.40 |
| ATOM | 5643 | CA  | ALA | 1462 | 77.240 | 79.227 | 30.767 | 1.00 | 23.17 |
| ATOM | 5644 | CB  | ALA | 1462 | 76.969 | 79.901 | 29.446 | 1.00 | 24.38 |
| ATOM | 5645 | C   | ALA | 1462 | 75.969 | 78.596 | 31.316 | 1.00 | 22.99 |
| ATOM | 5646 | O   | ALA | 1462 | 75.247 | 79.227 | 32.085 | 1.00 | 23.60 |
| ATOM | 5647 | N   | GLY | 1463 | 75.712 | 77.347 | 30.939 | 1.00 | 22.00 |
| ATOM | 5648 | CA  | GLY | 1463 | 74.524 | 76.655 | 31.404 | 1.00 | 20.76 |
| ATOM | 5649 | C   | GLY | 1463 | 74.563 | 76.411 | 32.893 | 1.00 | 21.18 |
| ATOM | 5650 | O   | GLY | 1463 | 73.586 | 76.670 | 33.595 | 1.00 | 22.33 |
| ATOM | 5651 | N   | ILE | 1464 | 75.707 | 75.935 | 33.376 | 1.00 | 21.45 |
| ATOM | 5652 | CA  | ILE | 1464 | 75.907 | 75.650 | 34.795 | 1.00 | 21.45 |
| ATOM | 5653 | CB  | ILE | 1464 | 77.279 | 74.972 | 35.048 | 1.00 | 17.77 |
| ATOM | 5654 | CG2 | ILE | 1464 | 77.472 | 74.652 | 36.525 | 1.00 | 16.84 |
| ATOM | 5655 | CG1 | ILE | 1464 | 77.375 | 73.672 | 34.263 | 1.00 | 12.39 |
| ATOM | 5656 | CD1 | ILE | 1464 | 78.696 | 72.995 | 34.442 | 1.00 | 21.13 |
| ATOM | 5657 | C   | ILE | 1464 | 75.819 | 76.933 | 35.621 | 1.00 | 24.69 |
| ATOM | 5658 | O   | ILE | 1464 | 75.201 | 76.948 | 36.693 | 1.00 | 27.98 |
| ATOM | 5659 | N   | GLN | 1465 | 76.420 | 78.010 | 35.115 | 1.00 | 23.43 |
| ATOM | 5660 | CA  | GLN | 1465 | 76.396 | 79.291 | 35.810 | 1.00 | 20.44 |
| ATOM | 5661 | CB  | GLN | 1465 | 77.198 | 80.333 | 35.046 | 1.00 | 20.47 |
| ATOM | 5662 | CG  | GLN | 1465 | 78.672 | 80.037 | 34.997 | 1.00 | 21.90 |
| ATOM | 5663 | CD  | GLN | 1465 | 79.479 | 81.241 | 34.585 | 1.00 | 23.86 |
| ATOM | 5664 | OE1 | GLN | 1465 | 80.564 | 81.483 | 35.108 | 1.00 | 24.24 |
| ATOM | 5665 | NE2 | GLN | 1465 | 78.944 | 82.019 | 33.655 | 1.00 | 25.91 |
| ATOM | 5666 | C   | GLN | 1465 | 74.977 | 79.790 | 36.029 | 1.00 | 19.83 |
| ATOM | 5667 | O   | GLN | 1465 | 74.672 | 80.390 | 37.060 | 1.00 | 20.11 |
| ATOM | 5668 | N   | HIS | 1466 | 74.106 | 79.557 | 35.058 | 1.00 | 20.26 |
| ATOM | 5669 | CA  | HIS | 1466 | 72.725 | 79.977 | 35.208 | 1.00 | 22.99 |
| ATOM | 5670 | CB  | HIS | 1466 | 71.998 | 79.979 | 33.873 | 1.00 | 24.47 |
| ATOM | 5671 | CG  | HIS | 1466 | 72.288 | 81.191 | 33.047 | 1.00 | 30.20 |
| ATOM | 5672 | CD2 | HIS | 1466 | 71.599 | 82.347 | 32.892 | 1.00 | 33.03 |
| ATOM | 5673 | ND1 | HIS | 1466 | 73.426 | 81.319 | 32.283 | 1.00 | 31.81 |
| ATOM | 5674 | CE1 | HIS | 1466 | 73.429 | 82.501 | 31.692 | 1.00 | 34.48 |
| ATOM | 5675 | NE2 | HIS | 1466 | 72.331 | 83.145 | 32.047 | 1.00 | 35.24 |
| ATOM | 5676 | C   | HIS | 1466 | 71.998 | 79.108 | 36.229 | 1.00 | 24.73 |
| ATOM | 5677 | O   | HIS | 1466 | 71.124 | 79.608 | 36.940 | 1.00 | 27.97 |
| ATOM | 5678 | N   | SER | 1467 | 72.363 | 77.826 | 36.328 | 1.00 | 22.87 |
| ATOM | 5679 | CA  | SER | 1467 | 71.734 | 76.941 | 37.307 | 1.00 | 21.98 |
| ATOM | 5680 | CB  | SER | 1467 | 72.240 | 75.510 | 37.173 | 1.00 | 19.47 |
| ATOM | 5681 | OG  | SER | 1467 | 71.817 | 74.941 | 35.958 | 1.00 | 25.92 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5682 | C   | SER | 1467 | 72.070 | 77.443 | 38.694 | 1.00 | 22.35 |
| ATOM | 5683 | O   | SER | 1467 | 71.182 | 77.701 | 39.502 | 1.00 | 26.52 |
| ATOM | 5684 | N   | CYS | 1468 | 73.361 | 77.616 | 38.950 | 1.00 | 21.86 |
| ATOM | 5685 | CA  | CYS | 1468 | 73.833 | 78.089 | 40.241 | 1.00 | 21.15 |
| ATOM | 5686 | CB  | CYS | 1468 | 75.349 | 78.280 | 40.219 | 1.00 | 19.89 |
| ATOM | 5687 | SG  | CYS | 1468 | 76.268 | 76.742 | 40.093 | 1.00 | 17.63 |
| ATOM | 5688 | C   | CYS | 1468 | 73.141 | 79.382 | 40.633 | 1.00 | 20.36 |
| ATOM | 5689 | O   | CYS | 1468 | 72.698 | 79.535 | 41.771 | 1.00 | 20.45 |
| ATOM | 5690 | N   | GLN | 1469 | 73.003 | 80.285 | 39.673 | 1.00 | 20.12 |
| ATOM | 5691 | CA  | GLN | 1469 | 72.351 | 81.554 | 39.927 | 1.00 | 20.40 |
| ATOM | 5692 | CB  | GLN | 1469 | 72.357 | 82.412 | 38.678 | 1.00 | 17.82 |
| ATOM | 5693 | CG  | GLN | 1469 | 71.694 | 83.733 | 38.897 | 1.00 | 17.81 |
| ATOM | 5694 | CD  | GLN | 1469 | 71.523 | 84.486 | 37.619 | 1.00 | 23.77 |
| ATOM | 5695 | OE1 | GLN | 1469 | 71.323 | 83.894 | 36.558 | 1.00 | 22.20 |
| ATOM | 5696 | NE2 | GLN | 1469 | 71.611 | 85.810 | 37.699 | 1.00 | 28.08 |
| ATOM | 5697 | C   | GLN | 1469 | 70.919 | 81.356 | 40.393 | 1.00 | 21.30 |
| ATOM | 5698 | O   | GLN | 1469 | 70.508 | 81.907 | 41.411 | 1.00 | 23.33 |
| ATOM | 5699 | N   | ASP | 1470 | 70.153 | 80.578 | 39.641 | 1.00 | 21.99 |
| ATOM | 5700 | CA  | ASP | 1470 | 68.771 | 80.323 | 40.004 | 1.00 | 22.24 |
| ATOM | 5701 | CB  | ASP | 1470 | 68.112 | 79.398 | 38.983 | 1.00 | 22.86 |
| ATOM | 5702 | CG  | ASP | 1470 | 67.573 | 80.146 | 37.766 | 1.00 | 25.39 |
| ATOM | 5703 | OD1 | ASP | 1470 | 67.784 | 81.375 | 37.639 | 1.00 | 21.98 |
| ATOM | 5704 | OD2 | ASP | 1470 | 66.913 | 79.488 | 36.937 | 1.00 | 24.95 |
| ATOM | 5705 | C   | ASP | 1470 | 68.664 | 79.731 | 41.401 | 1.00 | 22.03 |
| ATOM | 5706 | O   | ASP | 1470 | 67.805 | 80.139 | 42.187 | 1.00 | 22.26 |
| ATOM | 5707 | N   | ILE | 1471 | 69.564 | 78.807 | 41.726 | 1.00 | 21.04 |
| ATOM | 5708 | CA  | ILE | 1471 | 69.543 | 78.170 | 43.037 | 1.00 | 21.12 |
| ATOM | 5709 | CB  | ILE | 1471 | 70.160 | 76.725 | 43.012 | 1.00 | 22.81 |
| ATOM | 5710 | CG2 | ILE | 1471 | 69.450 | 75.859 | 41.976 | 1.00 | 19.90 |
| ATOM | 5711 | CG1 | ILE | 1471 | 71.653 | 76.755 | 42.689 | 1.00 | 25.14 |
| ATOM | 5712 | CD1 | ILE | 1471 | 72.284 | 75.374 | 42.600 | 1.00 | 21.70 |
| ATOM | 5713 | C   | ILE | 1471 | 70.160 | 79.040 | 44.139 | 1.00 | 20.42 |
| ATOM | 5714 | O   | ILE | 1471 | 70.011 | 78.739 | 45.324 | 1.00 | 20.93 |
| ATOM | 5715 | N   | GLY | 1472 | 70.808 | 80.137 | 43.751 | 1.00 | 19.66 |
| ATOM | 5716 | CA  | GLY | 1472 | 71.403 | 81.047 | 44.722 | 1.00 | 19.79 |
| ATOM | 5717 | C   | GLY | 1472 | 72.859 | 80.822 | 45.102 | 1.00 | 21.16 |
| ATOM | 5718 | O   | GLY | 1472 | 73.376 | 81.445 | 46.042 | 1.00 | 21.66 |
| ATOM | 5719 | N   | ALA | 1473 | 73.537 | 79.951 | 44.364 | 1.00 | 21.76 |
| ATOM | 5720 | CA  | ALA | 1473 | 74.932 | 79.640 | 44.631 | 1.00 | 21.14 |
| ATOM | 5721 | CB  | ALA | 1473 | 75.157 | 79.164 | 44.468 | 1.00 | 23.54 |
| ATOM | 5722 | C   | ALA | 1473 | 75.862 | 80.413 | 43.708 | 1.00 | 21.24 |
| ATOM | 5723 | O   | ALA | 1473 | 75.714 | 80.365 | 42.493 | 1.00 | 20.90 |
| ATOM | 5724 | N   | LYS | 1474 | 76.821 | 81.124 | 44.290 | 1.00 | 22.52 |
| ATOM | 5725 | CA  | LYS | 1474 | 77.783 | 81.903 | 43.516 | 1.00 | 23.89 |
| ATOM | 5726 | CB  | LYS | 1474 | 78.276 | 83.110 | 44.326 | 1.00 | 28.89 |
| ATOM | 5727 | CG  | LYS | 1474 | 77.167 | 84.009 | 44.856 | 1.00 | 38.03 |
| ATOM | 5728 | CD  | LYS | 1474 | 77.720 | 85.285 | 45.496 | 1.00 | 44.94 |
| ATOM | 5729 | CE  | LYS | 1474 | 76.605 | 86.167 | 46.073 | 1.00 | 47.23 |
| ATOM | 5730 | NZ  | LYS | 1474 | 75.848 | 85.496 | 47.173 | 1.00 | 49.89 |
| ATOM | 5731 | C   | LYS | 1474 | 78.983 | 81.057 | 43.110 | 1.00 | 22.37 |
| ATOM | 5732 | O   | LYS | 1474 | 79.919 | 81.561 | 42.506 | 1.00 | 23.41 |
| ATOM | 5733 | N   | SER | 1475 | 78.959 | 79.775 | 43.452 | 1.00 | 22.61 |
| ATOM | 5734 | CA  | SER | 1475 | 80.056 | 78.871 | 43.128 | 1.00 | 22.50 |
| ATOM | 5735 | CB  | SER | 1475 | 81.273 | 79.205 | 43.990 | 1.00 | 26.45 |
| ATOM | 5736 | OG  | SER | 1475 | 80.945 | 79.161 | 45.376 | 1.00 | 32.98 |
| ATOM | 5737 | C   | SER | 1475 | 79.645 | 77.430 | 43.393 | 1.00 | 21.22 |
| ATOM | 5738 | O   | SER | 1475 | 78.702 | 77.177 | 44.152 | 1.00 | 20.30 |
| ATOM | 5739 | N   | LEU | 1476 | 80.354 | 76.488 | 42.780 | 1.00 | 20.38 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5740 | CA  | LEU | 1476 | 80.051 | 75.077 | 42.987 | 1.00 | 18.61 |
| ATOM | 5741 | CB  | LEU | 1476 | 80.837 | 74.200 | 42.017 | 1.00 | 13.19 |
| ATOM | 5742 | CG  | LEU | 1476 | 80.552 | 74.458 | 40.530 | 1.00 | 9.83  |
| ATOM | 5743 | CD1 | LEU | 1476 | 81.212 | 73.391 | 39.698 | 1.00 | 6.72  |
| ATOM | 5744 | CD2 | LEU | 1476 | 79.066 | 74.458 | 40.248 | 1.00 | 9.78  |
| ATOM | 5745 | C   | LEU | 1476 | 80.297 | 74.670 | 44.443 | 1.00 | 18.33 |
| ATOM | 5746 | O   | LEU | 1476 | 79.567 | 73.858 | 44.997 | 1.00 | 21.64 |
| ATOM | 5747 | N   | THR | 1477 | 81.282 | 75.280 | 45.085 | 1.00 | 18.50 |
| ATOM | 5748 | CA  | THR | 1477 | 81.564 | 74.985 | 46.484 | 1.00 | 20.62 |
| ATOM | 5749 | CB  | THR | 1477 | 82.787 | 75.775 | 46.994 | 1.00 | 22.41 |
| ATOM | 5750 | OG1 | THR | 1477 | 83.954 | 75.394 | 46.249 | 1.00 | 24.52 |
| ATOM | 5751 | CG2 | THR | 1477 | 83.012 | 75.512 | 48.480 | 1.00 | 24.60 |
| ATOM | 5752 | C   | THR | 1477 | 80.352 | 75.394 | 47.315 | 1.00 | 21.09 |
| ATOM | 5753 | O   | THR | 1477 | 79.919 | 74.666 | 48.209 | 1.00 | 20.03 |
| ATOM | 5754 | N   | GLN | 1478 | 79.801 | 76.560 | 46.988 | 1.00 | 23.03 |
| ATOM | 5755 | CA  | GLN | 1478 | 78.633 | 77.097 | 47.682 | 1.00 | 21.72 |
| ATOM | 5756 | CB  | GLN | 1478 | 78.298 | 78.499 | 47.157 | 1.00 | 20.38 |
| ATOM | 5757 | CG  | GLN | 1478 | 77.346 | 79.323 | 48.022 | 1.00 | 22.66 |
| ATOM | 5758 | CD  | GLN | 1478 | 77.277 | 80.785 | 47.584 | 1.00 | 27.92 |
| ATOM | 5759 | OE1 | GLN | 1478 | 78.058 | 81.230 | 46.746 | 1.00 | 30.51 |
| ATOM | 5760 | NE2 | GLN | 1478 | 76.339 | 81.533 | 48.147 | 1.00 | 30.65 |
| ATOM | 5761 | C   | GLN | 1478 | 77.455 | 76.164 | 47.483 | 1.00 | 21.55 |
| ATOM | 5762 | O   | GLN | 1478 | 76.688 | 75.939 | 48.415 | 1.00 | 23.57 |
| ATOM | 5763 | N   | VAL | 1479 | 77.342 | 75.575 | 46.294 | 1.00 | 21.36 |
| ATOM | 5764 | CA  | VAL | 1479 | 76.233 | 74.660 | 46.017 | 1.00 | 21.51 |
| ATOM | 5765 | CB  | VAL | 1479 | 76.236 | 74.108 | 44.575 | 1.00 | 22.74 |
| ATOM | 5766 | CG1 | VAL | 1479 | 75.022 | 73.222 | 44.365 | 1.00 | 23.03 |
| ATOM | 5767 | CG2 | VAL | 1479 | 76.209 | 75.240 | 43.567 | 1.00 | 26.07 |
| ATOM | 5768 | C   | VAL | 1479 | 76.258 | 73.484 | 46.974 | 1.00 | 19.18 |
| ATOM | 5769 | O   | VAL | 1479 | 75.302 | 73.271 | 47.718 | 1.00 | 22.44 |
| ATOM | 5770 | N   | ARG | 1480 | 77.364 | 72.748 | 46.988 | 1.00 | 16.57 |
| ATOM | 5771 | CA  | ARG | 1480 | 77.491 | 71.593 | 47.872 | 1.00 | 15.29 |
| ATOM | 5772 | CB  | ARG | 1480 | 78.815 | 70.881 | 47.628 | 1.00 | 10.45 |
| ATOM | 5773 | CG  | ARG | 1480 | 78.930 | 70.342 | 46.217 | 1.00 | 9.69  |
| ATOM | 5774 | CD  | ARG | 1480 | 80.084 | 69.386 | 46.086 | 1.00 | 16.38 |
| ATOM | 5775 | NE  | ARG | 1480 | 81.362 | 70.000 | 46.434 | 1.00 | 21.07 |
| ATOM | 5776 | CZ  | ARG | 1480 | 82.036 | 70.818 | 45.632 | 1.00 | 25.55 |
| ATOM | 5777 | NH1 | ARG | 1480 | 81.551 | 71.129 | 44.433 | 1.00 | 27.33 |
| ATOM | 5778 | NH2 | ARG | 1480 | 83.198 | 71.322 | 46.026 | 1.00 | 26.79 |
| ATOM | 5779 | C   | ARG | 1480 | 77.343 | 71.961 | 49.345 | 1.00 | 16.36 |
| ATOM | 5780 | O   | ARG | 1480 | 76.749 | 71.215 | 50.121 | 1.00 | 18.23 |
| ATOM | 5781 | N   | ALA | 1481 | 77.855 | 73.126 | 49.724 | 1.00 | 17.05 |
| ATOM | 5782 | CA  | ALA | 1481 | 77.767 | 73.594 | 51.103 | 1.00 | 15.72 |
| ATOM | 5783 | CB  | ALA | 1481 | 78.547 | 74.874 | 51.265 | 1.00 | 14.94 |
| ATOM | 5784 | C   | ALA | 1481 | 76.311 | 73.811 | 51.507 | 1.00 | 16.85 |
| ATOM | 5785 | O   | ALA | 1481 | 75.902 | 73.446 | 52.612 | 1.00 | 16.33 |
| ATOM | 5786 | N   | MET | 1482 | 75.541 | 74.409 | 50.604 | 1.00 | 16.63 |
| ATOM | 5787 | CA  | MET | 1482 | 74.129 | 74.678 | 50.837 | 1.00 | 16.66 |
| ATOM | 5788 | CB  | MET | 1482 | 73.578 | 75.588 | 49.745 | 1.00 | 16.75 |
| ATOM | 5789 | CG  | MET | 1482 | 74.147 | 76.989 | 49.757 | 1.00 | 16.82 |
| ATOM | 5790 | SD  | MET | 1482 | 73.715 | 77.910 | 48.286 | 1.00 | 20.66 |
| ATOM | 5791 | CE  | MET | 1482 | 71.961 | 77.896 | 48.402 | 1.00 | 17.74 |
| ATOM | 5792 | C   | MET | 1482 | 73.327 | 73.386 | 50.867 | 1.00 | 17.97 |
| ATOM | 5793 | O   | MET | 1482 | 72.324 | 73.286 | 51.576 | 1.00 | 18.54 |
| ATOM | 5794 | N   | MET | 1483 | 73.753 | 72.404 | 50.081 | 1.00 | 16.86 |
| ATOM | 5795 | CA  | MET | 1483 | 73.061 | 71.126 | 50.046 | 1.00 | 18.50 |
| ATOM | 5796 | CB  | MET | 1483 | 73.510 | 70.306 | 48.832 | 1.00 | 20.94 |
| ATOM | 5797 | CG  | MET | 1483 | 72.920 | 68.905 | 48.753 | 1.00 | 21.75 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5798 | SD  | MET | 1483 | 74.049 | 67.613 | 49.328 | 1.00 | 25.70 |
| ATOM | 5799 | CE  | MET | 1483 | 73.300 | 67.145 | 50.866 | 1.00 | 28.55 |
| ATOM | 5800 | C   | MET | 1483 | 73.301 | 70.366 | 51.347 | 1.00 | 18.59 |
| ATOM | 5801 | O   | MET | 1483 | 72.349 | 70.004 | 52.041 | 1.00 | 19.17 |
| ATOM | 5802 | N   | TYR | 1484 | 74.569 | 70.174 | 51.703 | 1.00 | 17.46 |
| ATOM | 5803 | CA  | TYR | 1484 | 74.924 | 69.459 | 52.929 | 1.00 | 17.19 |
| ATOM | 5804 | CB  | TYR | 1484 | 76.447 | 69.295 | 53.052 | 1.00 | 14.82 |
| ATOM | 5805 | CG  | TYR | 1484 | 77.058 | 68.304 | 52.068 | 1.00 | 12.90 |
| ATOM | 5806 | CD1 | TYR | 1484 | 76.709 | 66.952 | 52.087 | 1.00 | 11.22 |
| ATOM | 5807 | CE1 | TYR | 1484 | 77.286 | 66.040 | 51.195 | 1.00 | 4.92  |
| ATOM | 5808 | CD2 | TYR | 1484 | 77.998 | 68.717 | 51.132 | 1.00 | 11.91 |
| ATOM | 5809 | CE2 | TYR | 1484 | 78.578 | 67.817 | 50.244 | 1.00 | 8.93  |
| ATOM | 5810 | CZ  | TYR | 1484 | 78.220 | 66.486 | 50.283 | 1.00 | 9.49  |
| ATOM | 5811 | OH  | TYR | 1484 | 78.824 | 65.617 | 49.411 | 1.00 | 16.42 |
| ATOM | 5812 | C   | TYR | 1484 | 74.342 | 70.094 | 54.196 | 1.00 | 17.55 |
| ATOM | 5813 | O   | TYR | 1484 | 73.985 | 69.386 | 55.137 | 1.00 | 20.47 |
| ATOM | 5814 | N   | SER | 1485 | 74.255 | 71.419 | 54.223 | 1.00 | 16.85 |
| ATOM | 5815 | CA  | SER | 1485 | 73.693 | 72.128 | 55.367 | 1.00 | 15.90 |
| ATOM | 5816 | CB  | SER | 1485 | 73.993 | 73.619 | 55.260 | 1.00 | 16.94 |
| ATOM | 5817 | OG  | SER | 1485 | 73.387 | 74.177 | 54.100 | 1.00 | 20.34 |
| ATOM | 5818 | C   | SER | 1485 | 72.185 | 71.943 | 55.375 | 1.00 | 16.36 |
| ATOM | 5819 | O   | SER | 1485 | 71.520 | 72.200 | 56.374 | 1.00 | 15.00 |
| ATOM | 5820 | N   | GLY | 1486 | 71.645 | 71.562 | 54.223 | 1.00 | 18.94 |
| ATOM | 5821 | CA  | GLY | 1486 | 70.213 | 71.363 | 54.101 | 1.00 | 19.06 |
| ATOM | 5822 | C   | GLY | 1486 | 69.528 | 72.559 | 53.469 | 1.00 | 20.47 |
| ATOM | 5823 | O   | GLY | 1486 | 68.349 | 72.482 | 53.105 | 1.00 | 21.02 |
| ATOM | 5824 | N   | GLU | 1487 | 70.268 | 73.655 | 53.306 | 1.00 | 19.69 |
| ATOM | 5825 | CA  | GLU | 1487 | 69.717 | 74.868 | 52.716 | 1.00 | 17.15 |
| ATOM | 5826 | CB  | GLU | 1487 | 70.761 | 75.970 | 52.669 | 1.00 | 15.86 |
| ATOM | 5827 | CG  | GLU | 1487 | 70.258 | 77.209 | 51.946 | 1.00 | 16.32 |
| ATOM | 5828 | CD  | GLU | 1487 | 71.152 | 78.412 | 52.111 | 1.00 | 17.63 |
| ATOM | 5829 | OE1 | GLU | 1487 | 72.336 | 78.241 | 52.488 | 1.00 | 21.20 |
| ATOM | 5830 | OE2 | GLU | 1487 | 70.658 | 79.536 | 51.866 | 1.00 | 20.22 |
| ATOM | 5831 | C   | GLU | 1487 | 69.131 | 74.669 | 51.325 | 1.00 | 17.26 |
| ATOM | 5832 | O   | GLU | 1487 | 68.021 | 75.127 | 51.053 | 1.00 | 18.70 |
| ATOM | 5833 | N   | LEU | 1488 | 69.901 | 74.056 | 50.431 | 1.00 | 15.56 |
| ATOM | 5834 | CA  | LEU | 1488 | 69.429 | 73.808 | 49.076 | 1.00 | 13.65 |
| ATOM | 5835 | CB  | LEU | 1488 | 70.553 | 73.244 | 48.207 | 1.00 | 10.67 |
| ATOM | 5836 | CG  | LEU | 1488 | 70.361 | 73.271 | 46.691 | 1.00 | 9.52  |
| ATOM | 5837 | CD1 | LEU | 1488 | 70.425 | 74.691 | 46.200 | 1.00 | 9.10  |
| ATOM | 5838 | CD2 | LEU | 1488 | 71.446 | 72.456 | 46.021 | 1.00 | 9.59  |
| ATOM | 5839 | C   | LEU | 1488 | 68.307 | 72.787 | 49.221 | 1.00 | 15.23 |
| ATOM | 5840 | O   | LEU | 1488 | 68.473 | 71.779 | 49.912 | 1.00 | 16.81 |
| ATOM | 5841 | N   | LYS | 1489 | 67.158 | 73.074 | 48.617 | 1.00 | 13.29 |
| ATOM | 5842 | CA  | LYS | 1489 | 66.008 | 72.186 | 48.695 | 1.00 | 12.48 |
| ATOM | 5843 | CB  | LYS | 1489 | 64.798 | 72.959 | 49.209 | 1.00 | 11.34 |
| ATOM | 5844 | CG  | LYS | 1489 | 64.876 | 73.337 | 50.681 | 1.00 | 11.57 |
| ATOM | 5845 | CD  | LYS | 1489 | 64.740 | 72.104 | 51.568 | 1.00 | 16.04 |
| ATOM | 5846 | CE  | LYS | 1489 | 64.503 | 72.469 | 53.025 | 1.00 | 15.13 |
| ATOM | 5847 | NZ  | LYS | 1489 | 65.702 | 73.077 | 53.666 | 1.00 | 18.46 |
| ATOM | 5848 | C   | LYS | 1489 | 65.694 | 71.562 | 47.344 | 1.00 | 13.92 |
| ATOM | 5849 | O   | LYS | 1489 | 65.850 | 72.208 | 46.310 | 1.00 | 15.51 |
| ATOM | 5850 | N   | PHE | 1490 | 65.249 | 70.307 | 47.366 | 1.00 | 14.08 |
| ATOM | 5851 | CA  | PHE | 1490 | 64.903 | 69.550 | 46.163 | 1.00 | 13.44 |
| ATOM | 5852 | CB  | PHE | 1490 | 65.772 | 68.304 | 46.044 | 1.00 | 13.69 |
| ATOM | 5853 | CG  | PHE | 1490 | 67.229 | 68.579 | 45.960 | 1.00 | 13.40 |
| ATOM | 5854 | CD1 | PHE | 1490 | 67.936 | 68.979 | 47.082 | 1.00 | 13.78 |
| ATOM | 5855 | CD2 | PHE | 1490 | 67.908 | 68.394 | 44.762 | 1.00 | 14.98 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5856 | CE1 | PHE | 1490 | 69.303 | 69.193 | 47.016 | 1.00 | 14.99 |
| ATOM | 5857 | CE2 | PHE | 1490 | 69.283 | 68.604 | 44.683 | 1.00 | 15.84 |
| ATOM | 5858 | CZ  | PHE | 1490 | 69.979 | 69.003 | 45.810 | 1.00 | 15.19 |
| ATOM | 5859 | C   | PHE | 1490 | 63.464 | 69.061 | 46.240 | 1.00 | 14.19 |
| ATOM | 5860 | O   | PHE | 1490 | 62.866 | 69.020 | 47.315 | 1.00 | 13.40 |
| ATOM | 5861 | N   | GLU | 1491 | 62.937 | 68.611 | 45.109 | 1.00 | 14.95 |
| ATOM | 5862 | CA  | GLU | 1491 | 61.585 | 68.072 | 45.062 | 1.00 | 16.53 |
| ATOM | 5863 | CB  | GLU | 1491 | 60.559 | 69.180 | 44.844 | 1.00 | 15.55 |
| ATOM | 5864 | CG  | GLU | 1491 | 59.148 | 68.662 | 44.957 | 1.00 | 15.94 |
| ATOM | 5865 | CD  | GLU | 1491 | 58.131 | 69.757 | 45.021 | 1.00 | 17.10 |
| ATOM | 5866 | OE1 | GLU | 1491 | 57.873 | 70.392 | 43.986 | 1.00 | 22.71 |
| ATOM | 5867 | OE2 | GLU | 1491 | 57.585 | 69.984 | 46.110 | 1.00 | 17.64 |
| ATOM | 5868 | C   | GLU | 1491 | 61.458 | 67.002 | 43.979 | 1.00 | 17.22 |
| ATOM | 5869 | O   | GLU | 1491 | 61.933 | 67.183 | 42.858 | 1.00 | 18.10 |
| ATOM | 5870 | N   | LYS | 1492 | 60.857 | 65.870 | 44.331 | 1.00 | 18.86 |
| ATOM | 5871 | CA  | LYS | 1492 | 60.675 | 64.771 | 43.385 | 1.00 | 20.24 |
| ATOM | 5872 | CB  | LYS | 1492 | 59.955 | 63.588 | 44.045 | 1.00 | 21.24 |
| ATOM | 5873 | CG  | LYS | 1492 | 60.671 | 62.965 | 45.228 | 1.00 | 29.14 |
| ATOM | 5874 | CD  | LYS | 1492 | 59.814 | 61.878 | 45.880 | 1.00 | 40.81 |
| ATOM | 5875 | CE  | LYS | 1492 | 60.384 | 61.403 | 47.225 | 1.00 | 47.79 |
| ATOM | 5876 | NZ  | LYS | 1492 | 59.540 | 60.341 | 47.876 | 1.00 | 51.47 |
| ATOM | 5877 | C   | LYS | 1492 | 59.863 | 65.245 | 42.189 | 1.00 | 21.19 |
| ATOM | 5878 | O   | LYS | 1492 | 59.241 | 66.304 | 42.225 | 1.00 | 22.42 |
| ATOM | 5879 | N   | ARG | 1493 | 59.812 | 64.418 | 41.155 | 1.00 | 22.65 |
| ATOM | 5880 | CA  | ARG | 1493 | 59.090 | 64.758 | 39.944 | 1.00 | 20.77 |
| ATOM | 5881 | CB  | ARG | 1493 | 60.090 | 65.283 | 38.907 | 1.00 | 17.58 |
| ATOM | 5882 | CG  | ARG | 1493 | 59.509 | 66.229 | 37.886 | 1.00 | 21.05 |
| ATOM | 5883 | CD  | ARG | 1493 | 60.557 | 67.199 | 37.349 | 1.00 | 13.84 |
| ATOM | 5884 | NE  | ARG | 1493 | 61.609 | 66.516 | 36.612 | 1.00 | 15.28 |
| ATOM | 5885 | CZ  | ARG | 1493 | 62.023 | 66.864 | 35.395 | 1.00 | 19.75 |
| ATOM | 5886 | NH1 | ARG | 1493 | 61.478 | 67.901 | 34.762 | 1.00 | 12.43 |
| ATOM | 5887 | NH2 | ARG | 1493 | 62.995 | 66.170 | 34.806 | 1.00 | 22.01 |
| ATOM | 5888 | C   | ARG | 1493 | 58.361 | 63.526 | 39.411 | 1.00 | 22.38 |
| ATOM | 5889 | O   | ARG | 1493 | 58.986 | 62.534 | 39.036 | 1.00 | 24.72 |
| ATOM | 5890 | N   | THR | 1494 | 57.035 | 63.554 | 39.460 | 1.00 | 21.33 |
| ATOM | 5891 | CA  | THR | 1494 | 56.240 | 62.449 | 38.938 | 1.00 | 17.93 |
| ATOM | 5892 | CB  | THR | 1494 | 54.767 | 62.647 | 39.278 | 1.00 | 13.07 |
| ATOM | 5893 | OG1 | THR | 1494 | 54.283 | 63.821 | 38.613 | 1.00 | 16.64 |
| ATOM | 5894 | CG2 | THR | 1494 | 54.590 | 62.840 | 40.758 | 1.00 | 9.17  |
| ATOM | 5895 | C   | THR | 1494 | 56.397 | 62.517 | 37.418 | 1.00 | 19.78 |
| ATOM | 5896 | O   | THR | 1494 | 56.855 | 63.534 | 36.893 | 1.00 | 21.83 |
| ATOM | 5897 | N   | SER | 1495 | 55.998 | 61.470 | 36.701 | 1.00 | 21.91 |
| ATOM | 5898 | CA  | SER | 1495 | 56.108 | 61.482 | 35.243 | 1.00 | 22.93 |
| ATOM | 5899 | CB  | SER | 1495 | 55.591 | 60.187 | 34.637 | 1.00 | 22.00 |
| ATOM | 5900 | OG  | SER | 1495 | 56.544 | 59.159 | 34.813 | 1.00 | 29.94 |
| ATOM | 5901 | C   | SER | 1495 | 55.356 | 62.665 | 34.653 | 1.00 | 25.21 |
| ATOM | 5902 | O   | SER | 1495 | 55.863 | 63.339 | 33.757 | 1.00 | 26.52 |
| ATOM | 5903 | N   | SER | 1496 | 54.151 | 62.922 | 35.154 | 1.00 | 25.45 |
| ATOM | 5904 | CA  | SER | 1496 | 53.376 | 64.056 | 34.681 | 1.00 | 24.09 |
| ATOM | 5905 | CB  | SER | 1496 | 52.026 | 64.125 | 35.397 | 1.00 | 24.76 |
| ATOM | 5906 | OG  | SER | 1496 | 51.146 | 63.121 | 34.928 | 1.00 | 24.43 |
| ATOM | 5907 | C   | SER | 1496 | 54.201 | 65.317 | 34.946 | 1.00 | 23.62 |
| ATOM | 5908 | O   | SER | 1496 | 54.329 | 66.172 | 34.071 | 1.00 | 26.31 |
| ATOM | 5909 | N   | ALA | 1497 | 54.811 | 65.405 | 36.125 | 1.00 | 20.98 |
| ATOM | 5910 | CA  | ALA | 1497 | 55.637 | 66.561 | 36.462 | 1.00 | 20.31 |
| ATOM | 5911 | CB  | ALA | 1497 | 56.022 | 66.526 | 37.931 | 1.00 | 20.07 |
| ATOM | 5912 | C   | ALA | 1497 | 56.885 | 66.612 | 35.564 | 1.00 | 19.59 |
| ATOM | 5913 | O   | ALA | 1497 | 57.508 | 67.665 | 35.404 | 1.00 | 18.61 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5914 | N   | GLN | 1498 | 57.244 | 65.469 | 34.985 | 1.00 | 18.72 |
| ATOM | 5915 | CA  | GLN | 1498 | 58.388 | 65.390 | 34.078 | 1.00 | 20.53 |
| ATOM | 5916 | CB  | GLN | 1498 | 58.963 | 63.965 | 34.035 | 1.00 | 22.06 |
| ATOM | 5917 | CG  | GLN | 1498 | 59.614 | 63.495 | 35.334 | 1.00 | 22.10 |
| ATOM | 5918 | CD  | GLN | 1498 | 60.314 | 62.146 | 35.192 | 1.00 | 24.33 |
| ATOM | 5919 | OE1 | GLN | 1498 | 60.366 | 61.348 | 36.136 | 1.00 | 28.22 |
| ATOM | 5920 | NE2 | GLN | 1498 | 60.864 | 61.890 | 34.018 | 1.00 | 25.10 |
| ATOM | 5921 | C   | GLN | 1498 | 57.959 | 65.822 | 32.668 | 1.00 | 19.53 |
| ATOM | 5922 | O   | GLN | 1498 | 58.644 | 66.610 | 32.011 | 1.00 | 17.18 |
| ATOM | 5923 | N   | VAL | 1499 | 56.807 | 65.327 | 32.225 | 1.00 | 19.64 |
| ATOM | 5924 | CA  | VAL | 1499 | 56.260 | 65.664 | 30.912 | 1.00 | 21.79 |
| ATOM | 5925 | CB  | VAL | 1499 | 54.935 | 64.916 | 30.648 | 1.00 | 24.74 |
| ATOM | 5926 | CG1 | VAL | 1499 | 54.392 | 65.273 | 29.271 | 1.00 | 28.60 |
| ATOM | 5927 | CG2 | VAL | 1499 | 55.146 | 63.416 | 30.752 | 1.00 | 23.82 |
| ATOM | 5928 | C   | VAL | 1499 | 55.989 | 67.165 | 30.866 | 1.00 | 21.34 |
| ATOM | 5929 | O   | VAL | 1499 | 56.251 | 67.836 | 29.871 | 1.00 | 20.70 |
| ATOM | 5930 | N   | GLU | 1500 | 55.469 | 67.679 | 31.970 | 1.00 | 23.11 |
| ATOM | 5931 | CA  | GLU | 1500 | 55.168 | 69.089 | 32.100 | 1.00 | 24.20 |
| ATOM | 5932 | CB  | GLU | 1500 | 54.407 | 69.337 | 33.397 | 1.00 | 21.44 |
| ATOM | 5933 | CG  | GLU | 1500 | 54.165 | 70.797 | 33.682 | 1.00 | 20.79 |
| ATOM | 5934 | CD  | GLU | 1500 | 53.539 | 71.018 | 35.029 | 1.00 | 22.34 |
| ATOM | 5935 | OE1 | GLU | 1500 | 54.295 | 71.197 | 36.010 | 1.00 | 19.52 |
| ATOM | 5936 | OE2 | GLU | 1500 | 52.289 | 71.013 | 35.109 | 1.00 | 25.92 |
| ATOM | 5937 | C   | GLU | 1500 | 56.439 | 69.931 | 32.093 | 1.00 | 26.10 |
| ATOM | 5938 | O   | GLU | 1500 | 56.414 | 71.097 | 31.692 | 1.00 | 29.46 |
| ATOM | 5939 | N   | GLY | 1501 | 57.529 | 69.361 | 32.594 | 1.00 | 25.56 |
| ATOM | 5940 | CA  | GLY | 1501 | 58.782 | 70.089 | 32.637 | 1.00 | 25.86 |
| ATOM | 5941 | C   | GLY | 1501 | 59.460 | 70.189 | 31.284 | 1.00 | 26.27 |
| ATOM | 5942 | O   | GLY | 1501 | 60.303 | 71.064 | 31.065 | 1.00 | 26.75 |
| ATOM | 5943 | N   | GLY | 1502 | 59.127 | 69.270 | 30.386 | 1.00 | 25.70 |
| ATOM | 5944 | CA  | GLY | 1502 | 59.720 | 69.302 | 29.066 | 1.00 | 24.56 |
| ATOM | 5945 | C   | GLY | 1502 | 58.752 | 69.921 | 28.084 | 1.00 | 24.73 |
| ATOM | 5946 | O   | GLY | 1502 | 57.611 | 70.224 | 28.444 | 1.00 | 24.99 |
| ATOM | 5947 | N   | VAL | 1503 | 59.192 | 70.112 | 26.846 | 1.00 | 23.11 |
| ATOM | 5948 | CA  | VAL | 1503 | 58.327 | 70.685 | 25.836 | 1.00 | 23.44 |
| ATOM | 5949 | CB  | VAL | 1503 | 59.041 | 70.797 | 24.492 | 1.00 | 19.90 |
| ATOM | 5950 | CG1 | VAL | 1503 | 58.095 | 71.365 | 23.450 | 1.00 | 21.64 |
| ATOM | 5951 | CG2 | VAL | 1503 | 60.264 | 71.678 | 24.637 | 1.00 | 14.59 |
| ATOM | 5952 | C   | VAL | 1503 | 57.092 | 69.798 | 25.697 | 1.00 | 27.31 |
| ATOM | 5953 | O   | VAL | 1503 | 57.186 | 68.568 | 25.736 | 1.00 | 27.96 |
| ATOM | 5954 | N   | HIS | 1504 | 55.932 | 70.429 | 25.558 | 1.00 | 28.89 |
| ATOM | 5955 | CA  | HIS | 1504 | 54.682 | 69.702 | 25.431 | 1.00 | 30.28 |
| ATOM | 5956 | CB  | HIS | 1504 | 54.257 | 69.149 | 26.799 | 1.00 | 26.93 |
| ATOM | 5957 | CG  | HIS | 1504 | 54.047 | 70.203 | 27.850 | 1.00 | 24.05 |
| ATOM | 5958 | CD2 | HIS | 1504 | 54.848 | 70.636 | 28.851 | 1.00 | 23.41 |
| ATOM | 5959 | ND1 | HIS | 1504 | 52.870 | 70.913 | 27.970 | 1.00 | 21.05 |
| ATOM | 5960 | CE1 | HIS | 1504 | 52.957 | 71.734 | 29.002 | 1.00 | 19.17 |
| ATOM | 5961 | NE2 | HIS | 1504 | 54.146 | 71.585 | 29.555 | 1.00 | 17.87 |
| ATOM | 5962 | C   | HIS | 1504 | 53.577 | 70.595 | 24.891 | 1.00 | 33.15 |
| ATOM | 5963 | O   | HIS | 1504 | 53.683 | 71.817 | 24.937 | 1.00 | 33.63 |
| ATOM | 5964 | N   | SER | 1505 | 52.527 | 69.971 | 24.363 | 1.00 | 36.01 |
| ATOM | 5965 | CA  | SER | 1505 | 51.355 | 70.683 | 23.855 | 1.00 | 39.13 |
| ATOM | 5966 | CB  | SER | 1505 | 50.766 | 71.540 | 24.978 | 1.00 | 41.06 |
| ATOM | 5967 | OG  | SER | 1505 | 50.603 | 70.761 | 26.158 | 1.00 | 43.13 |
| ATOM | 5968 | C   | SER | 1505 | 51.558 | 71.522 | 22.591 | 1.00 | 39.96 |
| ATOM | 5969 | O   | SER | 1505 | 50.737 | 72.391 | 22.268 | 1.00 | 42.24 |
| ATOM | 5970 | N   | LEU | 1506 | 52.625 | 71.228 | 21.858 | 1.00 | 38.97 |
| ATOM | 5971 | CA  | LEU | 1506 | 52.928 | 71.943 | 20.629 | 1.00 | 37.89 |

FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 5972 | CB  | LEU | 1506 | 54.389 | 72.400 | 20.626 | 1.00 | 34.20 |
| ATOM | 5973 | CG  | LEU | 1506 | 54.817 | 73.321 | 21.768 | 1.00 | 33.10 |
| ATOM | 5974 | CD1 | LEU | 1506 | 56.290 | 73.647 | 21.623 | 1.00 | 32.84 |
| ATOM | 5975 | CD2 | LEU | 1506 | 53.974 | 74.597 | 21.772 | 1.00 | 33.22 |
| ATOM | 5976 | C   | LEU | 1506 | 52.671 | 71.024 | 19.444 | 1.00 | 38.79 |
| ATOM | 5977 | O   | LEU | 1506 | 52.590 | 69.807 | 19.600 | 1.00 | 40.77 |
| ATOM | 5978 | N   | HIS | 1507 | 52.501 | 71.610 | 18.267 | 1.00 | 38.76 |
| ATOM | 5979 | CA  | HIS | 1507 | 52.277 | 70.833 | 17.064 | 1.00 | 38.33 |
| ATOM | 5980 | CB  | HIS | 1507 | 51.428 | 71.623 | 16.079 | 1.00 | 36.69 |
| ATOM | 5981 | CG  | HIS | 1507 | 51.148 | 70.886 | 14.812 | 1.00 | 37.52 |
| ATOM | 5982 | CD2 | HIS | 1507 | 51.836 | 70.819 | 13.649 | 1.00 | 36.79 |
| ATOM | 5983 | ND1 | HIS | 1507 | 50.062 | 70.054 | 14.668 | 1.00 | 39.80 |
| ATOM | 5984 | CE1 | HIS | 1507 | 50.093 | 69.501 | 13.467 | 1.00 | 42.20 |
| ATOM | 5985 | NE2 | HIS | 1507 | 51.160 | 69.950 | 12.828 | 1.00 | 39.42 |
| ATOM | 5986 | C   | HIS | 1507 | 53.628 | 70.488 | 16.436 | 1.00 | 40.28 |
| ATOM | 5987 | O   | HIS | 1507 | 53.735 | 69.574 | 15.619 | 1.00 | 41.56 |
| ATOM | 5988 | N   | SER | 1508 | 54.643 | 71.264 | 16.795 | 1.00 | 40.86 |
| ATOM | 5989 | CA  | SER | 1508 | 56.006 | 71.085 | 16.311 | 1.00 | 40.77 |
| ATOM | 5990 | CB  | SER | 1508 | 56.075 | 71.209 | 14.782 | 1.00 | 43.11 |
| ATOM | 5991 | OG  | SER | 1508 | 55.586 | 72.461 | 14.328 | 1.00 | 46.02 |
| ATOM | 5992 | C   | SER | 1508 | 56.818 | 72.186 | 16.963 | 1.00 | 40.37 |
| ATOM | 5993 | O   | SER | 1508 | 56.250 | 73.152 | 17.472 | 1.00 | 39.76 |
| ATOM | 5994 | N   | TYR | 1509 | 58.136 | 72.044 | 16.957 | 1.00 | 41.93 |
| ATOM | 5995 | CA  | TYR | 1509 | 59.001 | 73.037 | 17.569 | 1.00 | 44.96 |
| ATOM | 5996 | CB  | TYR | 1509 | 58.817 | 73.039 | 19.090 | 1.00 | 42.23 |
| ATOM | 5997 | CG  | TYR | 1509 | 59.187 | 71.736 | 19.772 | 1.00 | 40.95 |
| ATOM | 5998 | CD1 | TYR | 1509 | 58.297 | 70.663 | 19.800 | 1.00 | 40.13 |
| ATOM | 5999 | CE1 | TYR | 1509 | 58.621 | 69.474 | 20.452 | 1.00 | 39.44 |
| ATOM | 6000 | CD2 | TYR | 1509 | 60.420 | 71.587 | 20.411 | 1.00 | 39.93 |
| ATOM | 6001 | CE2 | TYR | 1509 | 60.755 | 70.403 | 21.065 | 1.00 | 37.74 |
| ATOM | 6002 | CZ  | TYR | 1509 | 59.852 | 69.350 | 21.084 | 1.00 | 37.07 |
| ATOM | 6003 | OH  | TYR | 1509 | 60.173 | 68.183 | 21.744 | 1.00 | 34.33 |
| ATOM | 6004 | C   | TYR | 1509 | 60.462 | 72.782 | 17.243 | 1.00 | 48.47 |
| ATOM | 6005 | O   | TYR | 1509 | 60.834 | 71.688 | 16.810 | 1.00 | 49.70 |
| ATOM | 6006 | N   | GLU | 1510 | 61.279 | 73.809 | 17.443 | 1.00 | 51.00 |
| ATOM | 6007 | CA  | GLU | 1510 | 62.709 | 73.723 | 17.213 | 1.00 | 53.89 |
| ATOM | 6008 | CB  | GLU | 1510 | 63.194 | 74.861 | 16.298 | 1.00 | 57.15 |
| ATOM | 6009 | CG  | GLU | 1510 | 62.659 | 74.847 | 14.866 | 1.00 | 63.16 |
| ATOM | 6010 | CD  | GLU | 1510 | 61.265 | 75.448 | 14.728 | 1.00 | 65.36 |
| ATOM | 6011 | OE1 | GLU | 1510 | 60.287 | 74.674 | 14.650 | 1.00 | 67.81 |
| ATOM | 6012 | OE2 | GLU | 1510 | 61.149 | 76.694 | 14.677 | 1.00 | 65.33 |
| ATOM | 6013 | C   | GLU | 1510 | 63.361 | 73.881 | 18.579 | 1.00 | 54.90 |
| ATOM | 6014 | O   | GLU | 1510 | 63.159 | 74.902 | 19.247 | 1.00 | 53.02 |
| ATOM | 6015 | N   | LYS | 1511 | 64.059 | 72.848 | 19.037 | 1.00 | 57.49 |
| ATOM | 6016 | CA  | LYS | 1511 | 64.748 | 72.939 | 20.316 | 1.00 | 61.49 |
| ATOM | 6017 | CB  | LYS | 1511 | 64.687 | 71.622 | 21.097 | 1.00 | 60.99 |
| ATOM | 6018 | CG  | LYS | 1511 | 65.450 | 71.678 | 22.425 | 1.00 | 61.77 |
| ATOM | 6019 | CD  | LYS | 1511 | 64.736 | 70.941 | 23.554 | 1.00 | 62.61 |
| ATOM | 6020 | CE  | LYS | 1511 | 64.610 | 69.451 | 23.290 | 1.00 | 62.49 |
| ATOM | 6021 | NZ  | LYS | 1511 | 63.891 | 68.781 | 24.404 | 1.00 | 59.52 |
| ATOM | 6022 | C   | LYS | 1511 | 66.184 | 73.322 | 19.989 | 1.00 | 64.39 |
| ATOM | 6023 | O   | LYS | 1511 | 66.991 | 72.475 | 19.609 | 1.00 | 64.69 |
| ATOM | 6024 | N   | ARG | 1512 | 66.462 | 74.621 | 20.073 | 1.00 | 67.99 |
| ATOM | 6025 | CA  | ARG | 1512 | 67.778 | 75.174 | 19.769 | 1.00 | 71.02 |
| ATOM | 6026 | CB  | ARG | 1512 | 67.660 | 76.148 | 18.587 | 1.00 | 72.88 |
| ATOM | 6027 | CG  | ARG | 1512 | 68.917 | 76.940 | 18.264 | 1.00 | 76.14 |
| ATOM | 6028 | CD  | ARG | 1512 | 68.686 | 77.854 | 17.070 | 1.00 | 77.65 |
| ATOM | 6029 | NE  | ARG | 1512 | 69.670 | 78.931 | 17.012 | 1.00 | 78.89 |



FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 6030 | CZ  | ARG | 1512 | 69.434 | 80.130 | 16.489 | 1.00 | 79.72 |
| ATOM | 6031 | NH1 | ARG | 1512 | 70.386 | 81.052 | 16.487 | 1.00 | 81.31 |
| ATOM | 6032 | NH2 | ARG | 1512 | 68.246 | 80.411 | 15.967 | 1.00 | 80.18 |
| ATOM | 6033 | C   | ARG | 1512 | 68.351 | 75.882 | 20.994 | 1.00 | 72.40 |
| ATOM | 6034 | O   | ARG | 1512 | 67.735 | 76.808 | 21.536 | 1.00 | 73.61 |
| ATOM | 6035 | N   | LEU | 1513 | 69.526 | 75.431 | 21.425 | 1.00 | 72.64 |
| ATOM | 6036 | CA  | LEU | 1513 | 70.202 | 75.995 | 22.589 | 1.00 | 72.96 |
| ATOM | 6037 | CB  | LEU | 1513 | 70.450 | 74.903 | 23.633 | 1.00 | 74.17 |
| ATOM | 6038 | CG  | LEU | 1513 | 69.907 | 75.114 | 25.046 | 1.00 | 75.57 |
| ATOM | 6039 | CD1 | LEU | 1513 | 70.459 | 76.390 | 25.644 | 1.00 | 74.67 |
| ATOM | 6040 | CD2 | LEU | 1513 | 68.403 | 75.154 | 25.002 | 1.00 | 76.98 |
| ATOM | 6041 | C   | LEU | 1513 | 71.540 | 76.569 | 22.157 | 1.00 | 72.37 |
| ATOM | 6042 | O   | LEU | 1513 | 72.330 | 75.870 | 21.524 | 1.00 | 74.72 |
| ATOM | 6043 | N   | PHE | 1514 | 71.786 | 77.831 | 22.493 | 1.00 | 70.03 |
| ATOM | 6044 | CA  | PHE | 1514 | 73.035 | 78.501 | 22.150 | 1.00 | 69.17 |
| ATOM | 6045 | CB  | PHE | 1514 | 74.187 | 77.962 | 23.022 | 1.00 | 68.65 |
| ATOM | 6046 | CG  | PHE | 1514 | 75.234 | 77.176 | 22.266 | 1.00 | 69.27 |
| ATOM | 6047 | CD1 | PHE | 1514 | 76.334 | 77.821 | 21.704 | 1.00 | 69.25 |
| ATOM | 6048 | CD2 | PHE | 1514 | 75.139 | 75.790 | 22.144 | 1.00 | 68.83 |
| ATOM | 6049 | CE1 | PHE | 1514 | 77.322 | 77.102 | 21.032 | 1.00 | 69.55 |
| ATOM | 6050 | CE2 | PHE | 1514 | 76.124 | 75.058 | 21.472 | 1.00 | 67.98 |
| ATOM | 6051 | CZ  | PHE | 1514 | 77.217 | 75.716 | 20.917 | 1.00 | 68.62 |
| ATOM | 6052 | C   | PHE | 1514 | 73.358 | 78.403 | 20.663 | 1.00 | 69.23 |
| ATOM | 6053 | O   | PHE | 1514 | 72.555 | 78.935 | 19.871 | 1.00 | 69.84 |

MYCOPHENOLIC ACID COORDINATES

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 6054 | C1  | MPA | 600  | 65.465 | 77.946 | 82.675 | 1.00 | 22.52 |
| ATOM | 6055 | C2  | MPA | 600  | 64.965 | 82.390 | 86.174 | 1.00 | 28.62 |
| ATOM | 6056 | C3  | MPA | 600  | 65.184 | 83.667 | 86.507 | 1.00 | 27.05 |
| ATOM | 6057 | C4  | MPA | 600  | 64.287 | 84.707 | 85.868 | 1.00 | 28.54 |
| ATOM | 6058 | C5  | MPA | 600  | 65.137 | 85.590 | 84.963 | 1.00 | 30.58 |
| ATOM | 6059 | C6  | MPA | 600  | 65.253 | 85.045 | 83.556 | 1.00 | 30.28 |
| ATOM | 6060 | C7  | MPA | 600  | 69.774 | 80.138 | 83.532 | 1.00 | 16.82 |
| ATOM | 6061 | C8  | MPA | 600  | 68.434 | 82.955 | 84.968 | 1.00 | 25.41 |
| ATOM | 6062 | C9  | MPA | 600  | 66.289 | 84.104 | 87.463 | 1.00 | 21.05 |
| ATOM | 6063 | C10 | MPA | 600  | 67.752 | 78.112 | 82.103 | 1.00 | 22.44 |
| ATOM | 6064 | C11 | MPA | 600  | 67.453 | 79.077 | 83.229 | 1.00 | 23.81 |
| ATOM | 6065 | C12 | MPA | 600  | 68.329 | 79.977 | 83.900 | 1.00 | 22.85 |
| ATOM | 6066 | C13 | MPA | 600  | 67.789 | 80.724 | 84.953 | 1.00 | 19.51 |
| ATOM | 6067 | C14 | MPA | 600  | 66.447 | 80.564 | 85.334 | 1.00 | 20.51 |
| ATOM | 6068 | C15 | MPA | 600  | 65.599 | 79.682 | 84.658 | 1.00 | 21.29 |
| ATOM | 6069 | C16 | MPA | 600  | 66.128 | 78.943 | 83.588 | 1.00 | 20.87 |
| ATOM | 6070 | C17 | MPA | 600  | 65.922 | 81.277 | 86.548 | 1.00 | 26.71 |
| ATOM | 6071 | O1  | MPA | 600  | 64.326 | 77.614 | 82.588 | 1.00 | 24.71 |
| ATOM | 6072 | O2  | MPA | 600  | 66.444 | 77.474 | 81.897 | 1.00 | 22.84 |
| ATOM | 6073 | O3  | MPA | 600  | 68.589 | 81.644 | 85.549 | 1.00 | 22.76 |
| ATOM | 6074 | O4  | MPA | 600  | 64.288 | 79.552 | 85.100 | 1.00 | 22.58 |
| ATOM | 6075 | O5  | MPA | 600  | 64.203 | 84.705 | 82.966 | 1.00 | 29.39 |
| ATOM | 6076 | O6  | MPA | 600  | 66.393 | 84.955 | 83.045 | 1.00 | 26.99 |
| ATOM | 6077 | C1  | MPA | 1600 | 79.693 | 50.178 | 33.345 | 1.00 | 26.44 |
| ATOM | 6078 | C2  | MPA | 1600 | 83.159 | 47.108 | 29.935 | 1.00 | 29.82 |
| ATOM | 6079 | C3  | MPA | 1600 | 84.293 | 46.491 | 29.575 | 1.00 | 34.15 |
| ATOM | 6080 | C4  | MPA | 1600 | 84.532 | 45.067 | 30.003 | 1.00 | 37.23 |
| ATOM | 6081 | C5  | MPA | 1600 | 85.484 | 45.043 | 31.192 | 1.00 | 40.84 |
| ATOM | 6082 | C6  | MPA | 1600 | 84.826 | 45.492 | 32.482 | 1.00 | 44.96 |
| ATOM | 6083 | C7  | MPA | 1600 | 84.075 | 52.238 | 32.906 | 1.00 | 17.32 |

# FIGURE 1 (CONT.)

|      |      |     |     |      |        |        |        |      |       |
|------|------|-----|-----|------|--------|--------|--------|------|-------|
| ATOM | 6084 | C8  | MPA | 1600 | 85.729 | 49.609 | 31.502 | 1.00 | 27.67 |
| ATOM | 6085 | C9  | MPA | 1600 | 85.387 | 47.148 | 28.760 | 1.00 | 35.11 |
| ATOM | 6086 | C10 | MPA | 1600 | 81.252 | 51.809 | 34.093 | 1.00 | 28.90 |
| ATOM | 6087 | C11 | MPA | 1600 | 81.874 | 51.061 | 32.928 | 1.00 | 26.34 |
| ATOM | 6088 | C12 | MPA | 1600 | 83.142 | 51.217 | 32.355 | 1.00 | 22.18 |
| ATOM | 6089 | C13 | MPA | 1600 | 83.489 | 50.344 | 31.304 | 1.00 | 24.79 |
| ATOM | 6090 | C14 | MPA | 1600 | 82.574 | 49.363 | 30.850 | 1.00 | 26.59 |
| ATOM | 6091 | C15 | MPA | 1600 | 81.294 | 49.201 | 31.461 | 1.00 | 29.67 |
| ATOM | 6092 | C16 | MPA | 1600 | 80.967 | 50.093 | 32.513 | 1.00 | 28.76 |
| ATOM | 6093 | C17 | MPA | 1600 | 82.921 | 48.553 | 29.618 | 1.00 | 25.16 |
| ATOM | 6094 | O1  | MPA | 1600 | 78.656 | 49.607 | 33.246 | 1.00 | 25.25 |
| ATOM | 6095 | O2  | MPA | 1600 | 79.927 | 51.146 | 34.238 | 1.00 | 27.50 |
| ATOM | 6096 | O3  | MPA | 1600 | 84.766 | 50.358 | 30.746 | 1.00 | 26.41 |
| ATOM | 6097 | O4  | MPA | 1600 | 80.486 | 48.095 | 31.123 | 1.00 | 27.52 |
| ATOM | 6098 | O5  | MPA | 1600 | 83.932 | 44.764 | 32.975 | 1.00 | 45.51 |
| ATOM | 6099 | O6  | MPA | 1600 | 85.195 | 46.576 | 33.001 | 1.00 | 44.94 |

## POTASSIUM ION COORDINATES

|      |      |   |     |     |        |        |        |      |       |
|------|------|---|-----|-----|--------|--------|--------|------|-------|
| ATOM | 6100 | K | POT | 601 | 63.503 | 70.962 | 85.991 | 1.00 | 41.47 |
| ATOM | 6101 | K | POT | 602 | 72.494 | 52.620 | 29.752 | 1.00 | 37.46 |

## WATER MOLECULE COORDINATES

|      |      |     |      |     |        |        |         |      |       |
|------|------|-----|------|-----|--------|--------|---------|------|-------|
| ATOM | 6102 | OH2 | TIP3 | 603 | 63.529 | 79.256 | 47.792  | 1.00 | 13.93 |
| ATOM | 6103 | OH2 | TIP3 | 604 | 91.351 | 74.319 | 96.225  | 1.00 | 20.69 |
| ATOM | 6104 | OH2 | TIP3 | 605 | 72.344 | 46.035 | 101.631 | 1.00 | 17.67 |
| ATOM | 6105 | OH2 | TIP3 | 606 | 85.033 | 54.784 | 29.616  | 1.00 | 20.16 |
| ATOM | 6106 | OH2 | TIP3 | 607 | 96.774 | 41.059 | 42.265  | 1.00 | 21.27 |
| ATOM | 6107 | OH2 | TIP3 | 608 | 64.807 | 62.160 | 83.369  | 1.00 | 22.21 |
| ATOM | 6108 | OH2 | TIP3 | 609 | 74.275 | 63.885 | 63.004  | 1.00 | 27.93 |
| ATOM | 6109 | OH2 | TIP3 | 610 | 87.085 | 56.492 | 64.953  | 1.00 | 59.52 |
| ATOM | 6110 | OH2 | TIP3 | 611 | 68.730 | 96.796 | 74.318  | 1.00 | 25.43 |
| ATOM | 6111 | OH2 | TIP3 | 612 | 91.223 | 66.176 | 88.226  | 1.00 | 23.25 |
| ATOM | 6112 | OH2 | TIP3 | 613 | 66.928 | 74.617 | 83.416  | 1.00 | 21.39 |
| ATOM | 6113 | OH2 | TIP3 | 614 | 71.384 | 87.659 | 97.919  | 1.00 | 52.73 |
| ATOM | 6114 | OH2 | TIP3 | 615 | 70.964 | 58.275 | 81.606  | 1.00 | 37.09 |
| ATOM | 6115 | OH2 | TIP3 | 616 | 66.840 | 52.566 | 68.535  | 1.00 | 30.80 |
| ATOM | 6116 | OH2 | TIP3 | 617 | 72.339 | 79.150 | 86.746  | 1.00 | 26.56 |
| ATOM | 6117 | OH2 | TIP3 | 618 | 77.701 | 57.856 | 53.021  | 1.00 | 59.36 |
| ATOM | 6118 | OH2 | TIP3 | 619 | 88.760 | 76.344 | 71.423  | 1.00 | 25.83 |
| ATOM | 6119 | OH2 | TIP3 | 620 | 85.731 | 78.904 | 27.766  | 1.00 | 53.37 |
| ATOM | 6120 | OH2 | TIP3 | 621 | 92.864 | 86.761 | 83.337  | 1.00 | 50.40 |
| ATOM | 6121 | OH2 | TIP3 | 622 | 52.798 | 60.668 | 36.659  | 1.00 | 44.29 |
| ATOM | 6122 | OH2 | TIP3 | 623 | 90.156 | 46.925 | 37.917  | 1.00 | 54.24 |
| ATOM | 6123 | OH2 | TIP3 | 624 | 66.346 | 64.284 | 84.367  | 1.00 | 41.00 |
| ATOM | 6124 | OH2 | TIP3 | 625 | 78.607 | 68.770 | 56.915  | 1.00 | 48.73 |
| ATOM | 6125 | OH2 | TIP3 | 626 | 85.421 | 51.000 | 81.149  | 1.00 | 29.22 |
| ATOM | 6126 | OH2 | TIP3 | 627 | 81.905 | 76.656 | 101.724 | 1.00 | 40.26 |
| ATOM | 6127 | OH2 | TIP3 | 628 | 69.287 | 88.078 | 78.412  | 1.00 | 41.23 |
| ATOM | 6128 | OH2 | TIP3 | 629 | 79.428 | 72.947 | 68.392  | 1.00 | 18.91 |
| ATOM | 6129 | OH2 | TIP3 | 630 | 68.417 | 98.204 | 82.153  | 1.00 | 40.95 |
| ATOM | 6130 | OH2 | TIP3 | 631 | 74.926 | 65.022 | 60.600  | 1.00 | 56.88 |
| ATOM | 6131 | OH2 | TIP3 | 632 | 97.224 | 50.021 | 75.346  | 1.00 | 35.64 |
| ATOM | 6132 | OH2 | TIP3 | 633 | 71.296 | 88.279 | 64.915  | 1.00 | 54.34 |
| ATOM | 6133 | OH2 | TIP3 | 634 | 80.899 | 65.865 | 59.607  | 1.00 | 32.10 |

FIGURE 1 (CONT.)

|      |      |     |      |     |         |        |         |      |       |
|------|------|-----|------|-----|---------|--------|---------|------|-------|
| ATOM | 6134 | OH2 | TIP3 | 635 | 66.483  | 65.049 | 30.246  | 1.00 | 20.26 |
| ATOM | 6135 | OH2 | TIP3 | 636 | 93.787  | 75.011 | 36.209  | 1.00 | 40.10 |
| ATOM | 6136 | OH2 | TIP3 | 637 | 83.837  | 45.961 | 49.613  | 1.00 | 30.53 |
| ATOM | 6137 | OH2 | TIP3 | 638 | 110.170 | 56.656 | 42.696  | 1.00 | 41.92 |
| ATOM | 6138 | OH2 | TIP3 | 639 | 84.500  | 64.574 | 47.772  | 1.00 | 42.47 |
| ATOM | 6139 | OH2 | TIP3 | 640 | 84.650  | 68.995 | 68.569  | 1.00 | 22.92 |
| ATOM | 6140 | OH2 | TIP3 | 641 | 75.389  | 62.003 | 106.019 | 1.00 | 64.07 |
| ATOM | 6141 | OH2 | TIP3 | 642 | 65.093  | 83.895 | 66.370  | 1.00 | 35.20 |
| ATOM | 6142 | OH2 | TIP3 | 643 | 79.572  | 69.513 | 68.092  | 1.00 | 41.73 |
| ATOM | 6143 | OH2 | TIP3 | 644 | 81.705  | 69.807 | 13.345  | 1.00 | 75.61 |
| ATOM | 6144 | OH2 | TIP3 | 645 | 79.766  | 83.945 | 66.824  | 1.00 | 38.58 |
| ATOM | 6145 | OH2 | TIP3 | 646 | 76.630  | 91.036 | 98.006  | 1.00 | 30.86 |
| ATOM | 6146 | OH2 | TIP3 | 647 | 92.426  | 72.749 | 82.096  | 1.00 | 23.28 |
| ATOM | 6147 | OH2 | TIP3 | 648 | 92.577  | 69.692 | 44.133  | 1.00 | 36.85 |
| ATOM | 6148 | OH2 | TIP3 | 649 | 82.576  | 41.782 | 29.517  | 1.00 | 39.32 |
| ATOM | 6149 | OH2 | TIP3 | 650 | 65.551  | 66.516 | 32.182  | 1.00 | 34.30 |
| ATOM | 6150 | OH2 | TIP3 | 651 | 61.739  | 81.979 | 81.423  | 1.00 | 21.79 |
| ATOM | 6151 | OH2 | TIP3 | 652 | 74.532  | 61.047 | 62.982  | 1.00 | 23.13 |
| ATOM | 6152 | OH2 | TIP3 | 653 | 73.416  | 69.959 | 84.520  | 1.00 | 24.72 |
| ATOM | 6153 | OH2 | TIP3 | 654 | 87.526  | 78.696 | 87.501  | 1.00 | 28.42 |
| ATOM | 6154 | OH2 | TIP3 | 655 | 73.301  | 97.166 | 75.481  | 1.00 | 29.52 |
| ATOM | 6155 | OH2 | TIP3 | 656 | 80.797  | 97.236 | 80.169  | 1.00 | 36.44 |
| ATOM | 6156 | OH2 | TIP3 | 657 | 72.410  | 82.003 | 80.433  | 1.00 | 39.64 |
| ATOM | 6157 | OH2 | TIP3 | 658 | 70.797  | 81.205 | 86.943  | 1.00 | 26.15 |
| ATOM | 6158 | OH2 | TIP3 | 659 | 69.119  | 86.448 | 85.434  | 1.00 | 37.81 |
| ATOM | 6159 | OH2 | TIP3 | 660 | 65.869  | 78.967 | 75.344  | 1.00 | 39.42 |
| ATOM | 6160 | OH2 | TIP3 | 661 | 87.122  | 84.588 | 70.107  | 1.00 | 41.94 |
| ATOM | 6161 | OH2 | TIP3 | 662 | 66.313  | 71.983 | 78.252  | 1.00 | 15.40 |
| ATOM | 6162 | OH2 | TIP3 | 663 | 61.479  | 73.532 | 84.529  | 1.00 | 24.10 |
| ATOM | 6163 | OH2 | TIP3 | 664 | 73.933  | 69.027 | 88.128  | 1.00 | 25.97 |
| ATOM | 6164 | OH2 | TIP3 | 665 | 63.498  | 69.506 | 79.814  | 1.00 | 26.48 |
| ATOM | 6165 | OH2 | TIP3 | 666 | 61.100  | 68.368 | 79.010  | 1.00 | 45.05 |
| ATOM | 6166 | OH2 | TIP3 | 667 | 73.033  | 68.873 | 79.995  | 1.00 | 10.40 |
| ATOM | 6167 | OH2 | TIP3 | 668 | 75.053  | 67.738 | 67.556  | 1.00 | 25.98 |
| ATOM | 6168 | OH2 | TIP3 | 669 | 70.945  | 65.926 | 61.108  | 1.00 | 30.20 |
| ATOM | 6169 | OH2 | TIP3 | 670 | 79.966  | 71.965 | 70.861  | 1.00 | 14.26 |
| ATOM | 6170 | OH2 | TIP3 | 671 | 73.205  | 58.622 | 82.862  | 1.00 | 34.10 |
| ATOM | 6171 | OH2 | TIP3 | 672 | 77.591  | 58.927 | 88.294  | 1.00 | 31.75 |
| ATOM | 6172 | OH2 | TIP3 | 673 | 82.216  | 67.818 | 102.675 | 1.00 | 31.66 |
| ATOM | 6173 | OH2 | TIP3 | 674 | 82.356  | 73.417 | 96.074  | 1.00 | 45.06 |
| ATOM | 6174 | OH2 | TIP3 | 675 | 74.350  | 76.446 | 100.156 | 1.00 | 20.12 |
| ATOM | 6175 | OH2 | TIP3 | 676 | 73.281  | 74.984 | 103.568 | 1.00 | 37.74 |
| ATOM | 6176 | OH2 | TIP3 | 677 | 67.784  | 70.872 | 110.507 | 1.00 | 50.41 |
| ATOM | 6177 | OH2 | TIP3 | 678 | 78.658  | 70.113 | 110.447 | 1.00 | 37.54 |
| ATOM | 6178 | OH2 | TIP3 | 679 | 68.600  | 84.196 | 101.581 | 1.00 | 67.03 |
| ATOM | 6179 | OH2 | TIP3 | 680 | 68.093  | 85.770 | 90.932  | 1.00 | 32.35 |
| ATOM | 6180 | OH2 | TIP3 | 681 | 60.473  | 85.655 | 86.947  | 1.00 | 34.10 |
| ATOM | 6181 | OH2 | TIP3 | 682 | 84.197  | 63.598 | 97.245  | 1.00 | 34.52 |
| ATOM | 6182 | OH2 | TIP3 | 683 | 90.212  | 55.985 | 83.506  | 1.00 | 56.22 |
| ATOM | 6183 | OH2 | TIP3 | 684 | 88.466  | 52.166 | 69.315  | 1.00 | 46.13 |
| ATOM | 6184 | OH2 | TIP3 | 685 | 93.732  | 59.819 | 73.153  | 1.00 | 29.48 |
| ATOM | 6185 | OH2 | TIP3 | 686 | 74.318  | 60.741 | 59.818  | 1.00 | 33.51 |
| ATOM | 6186 | OH2 | TIP3 | 687 | 84.856  | 56.311 | 60.236  | 1.00 | 55.85 |
| ATOM | 6187 | OH2 | TIP3 | 688 | 75.504  | 58.569 | 65.142  | 1.00 | 24.35 |
| ATOM | 6188 | OH2 | TIP3 | 689 | 66.245  | 47.634 | 93.849  | 1.00 | 35.24 |
| ATOM | 6189 | OH2 | TIP3 | 690 | 88.810  | 54.683 | 17.033  | 1.00 | 68.14 |
| ATOM | 6190 | OH2 | TIP3 | 691 | 83.094  | 60.169 | 17.837  | 1.00 | 42.20 |
| ATOM | 6191 | OH2 | TIP3 | 692 | 92.231  | 70.264 | 19.371  | 1.00 | 22.36 |

FIGURE 1 (CONT.)

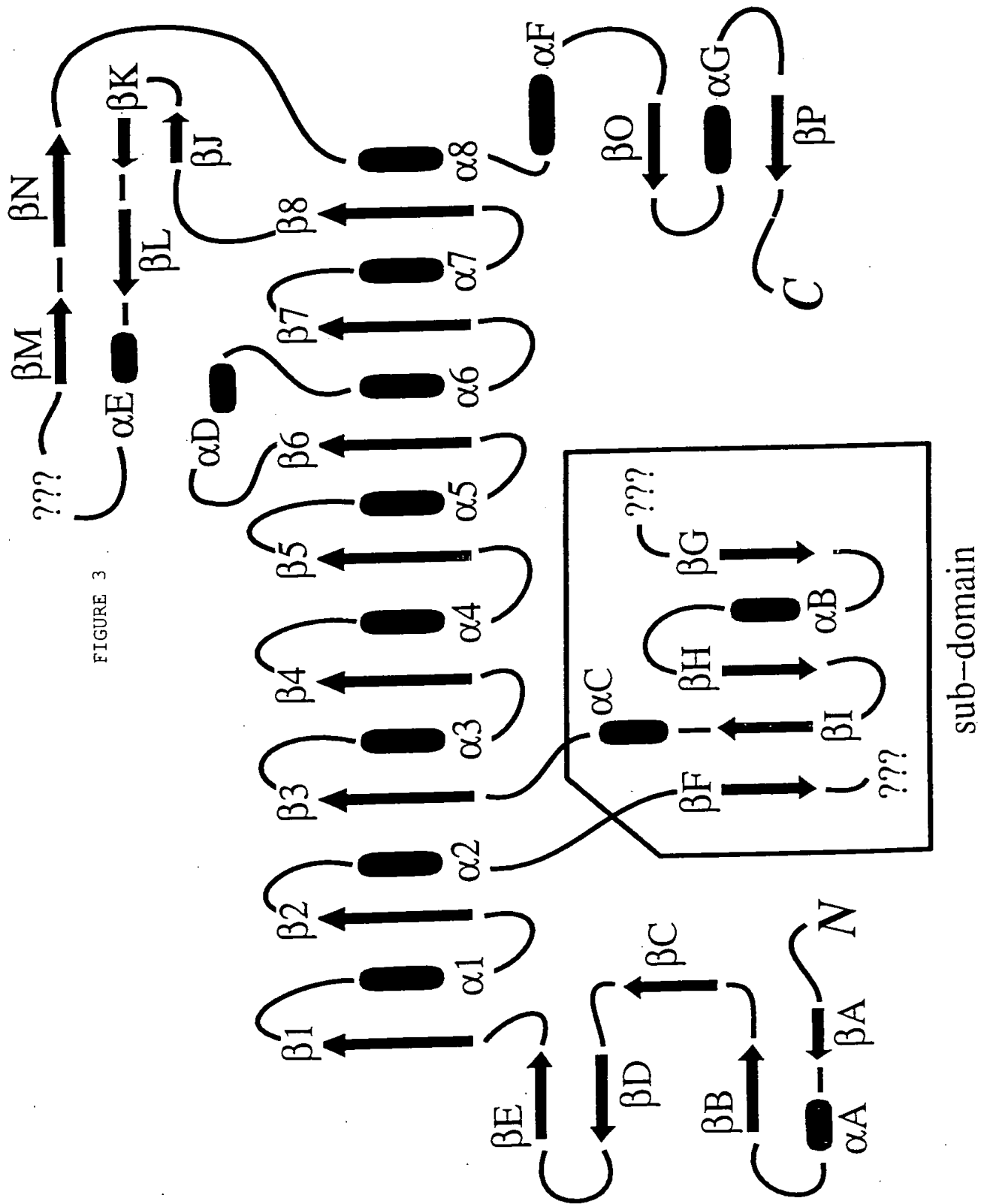
|      |      |     |      |     |         |        |         |      |        |
|------|------|-----|------|-----|---------|--------|---------|------|--------|
| ATOM | 6192 | OH2 | TIP3 | 693 | 89.874  | 79.054 | 28.213  | 1.00 | 23.97  |
| ATOM | 6193 | OH2 | TIP3 | 694 | 93.455  | 67.246 | 28.718  | 1.00 | 19.81  |
| ATOM | 6194 | OH2 | TIP3 | 695 | 104.670 | 51.741 | 36.100  | 1.00 | 54.63  |
| ATOM | 6195 | OH2 | TIP3 | 696 | 80.782  | 44.301 | 34.548  | 1.00 | 31.71  |
| ATOM | 6196 | OH2 | TIP3 | 697 | 81.029  | 45.306 | 48.967  | 1.00 | 21.33  |
| ATOM | 6197 | OH2 | TIP3 | 698 | 97.717  | 63.697 | 46.528  | 1.00 | 47.29  |
| ATOM | 6198 | OH2 | TIP3 | 699 | 93.154  | 58.370 | 49.439  | 1.00 | 29.43  |
| ATOM | 6199 | OH2 | TIP3 | 700 | 73.721  | 49.371 | 31.619  | 1.00 | 28.64  |
| ATOM | 6200 | OH2 | TIP3 | 701 | 75.341  | 54.478 | 37.368  | 1.00 | 44.88  |
| ATOM | 6201 | OH2 | TIP3 | 702 | 71.483  | 53.761 | 36.481  | 1.00 | 43.75  |
| ATOM | 6202 | OH2 | TIP3 | 703 | 70.805  | 48.134 | 29.440  | 1.00 | 45.27  |
| ATOM | 6203 | OH2 | TIP3 | 704 | 67.240  | 57.027 | 45.672  | 1.00 | 23.68  |
| ATOM | 6204 | OH2 | TIP3 | 705 | 73.938  | 65.367 | 53.641  | 1.00 | 35.21  |
| ATOM | 6205 | OH2 | TIP3 | 706 | 76.765  | 63.952 | 48.838  | 1.00 | 39.11  |
| ATOM | 6206 | OH2 | TIP3 | 707 | 86.429  | 64.888 | 41.271  | 1.00 | 47.43  |
| ATOM | 6207 | OH2 | TIP3 | 708 | 79.337  | 55.169 | 33.298  | 1.00 | 25.21  |
| ATOM | 6208 | OH2 | TIP3 | 709 | 77.021  | 61.621 | 35.635  | 1.00 | 12.75  |
| ATOM | 6209 | OH2 | TIP3 | 710 | 77.475  | 62.445 | 28.068  | 1.00 | 17.76  |
| ATOM | 6210 | OH2 | TIP3 | 711 | 65.308  | 68.280 | 34.978  | 1.00 | 60.08  |
| ATOM | 6211 | OH2 | TIP3 | 712 | 81.233  | 66.515 | 47.960  | 1.00 | 16.11  |
| ATOM | 6212 | OH2 | TIP3 | 713 | 85.329  | 69.050 | 46.064  | 1.00 | 41.01  |
| ATOM | 6213 | OH2 | TIP3 | 714 | 78.087  | 61.162 | 31.841  | 1.00 | 33.88  |
| ATOM | 6214 | OH2 | TIP3 | 715 | 83.936  | 58.250 | 16.183  | 1.00 | 19.59  |
| ATOM | 6215 | OH2 | TIP3 | 716 | 84.076  | 55.186 | 22.421  | 1.00 | 52.59  |
| ATOM | 6216 | OH2 | TIP3 | 717 | 71.928  | 61.664 | 18.579  | 1.00 | 20.02  |
| ATOM | 6217 | OH2 | TIP3 | 718 | 71.233  | 71.762 | 28.181  | 1.00 | 52.28  |
| ATOM | 6218 | OH2 | TIP3 | 719 | 82.842  | 72.092 | 48.741  | 1.00 | 29.08  |
| ATOM | 6219 | OH2 | TIP3 | 720 | 66.512  | 75.646 | 47.219  | 1.00 | 30.30  |
| ATOM | 6220 | OH2 | TIP3 | 721 | 47.558  | 69.374 | 15.382  | 1.00 | 63.67  |
| ATOM | 6221 | OH2 | TIP3 | 722 | 57.528  | 74.361 | 14.349  | 1.00 | 17.13  |
| ATOM | 6222 | OH2 | TIP3 | 723 | 92.602  | 74.600 | 98.553  | 1.00 | 40.55  |
| ATOM | 6223 | OH2 | TIP3 | 724 | 95.012  | 73.669 | 97.163  | 1.00 | 52.61  |
| ATOM | 6224 | OH2 | TIP3 | 725 | 85.703  | 52.369 | 29.241  | 1.00 | 33.33  |
| ATOM | 6225 | OH2 | TIP3 | 726 | 87.263  | 53.317 | 35.120  | 1.00 | 33.57  |
| ATOM | 6226 | OH2 | TIP3 | 727 | 97.146  | 44.242 | 39.694  | 1.00 | 51.07  |
| ATOM | 6227 | OH2 | TIP3 | 728 | 66.879  | 61.968 | 81.685  | 1.00 | 21.70  |
| ATOM | 6228 | OH2 | TIP3 | 729 | 63.716  | 59.555 | 84.121  | 1.00 | 19.58  |
| ATOM | 6229 | OH2 | TIP3 | 730 | 68.397  | 64.441 | 82.651  | 1.00 | 40.07  |
| ATOM | 6230 | OH2 | TIP3 | 731 | 71.867  | 59.240 | 59.629  | 1.00 | 50.06  |
| ATOM | 6231 | OH2 | TIP3 | 732 | 89.666  | 54.437 | 68.351  | 1.00 | 47.64  |
| ATOM | 6232 | OH2 | TIP3 | 733 | 71.067  | 95.544 | 76.431  | 1.00 | 60.59  |
| ATOM | 6233 | OH2 | TIP3 | 734 | 65.904  | 98.120 | 73.267  | 1.00 | 71.60  |
| ATOM | 6234 | OH2 | TIP3 | 735 | 92.274  | 63.420 | 87.295  | 1.00 | 34.70  |
| ATOM | 6235 | OH2 | TIP3 | 736 | 91.884  | 59.474 | 86.045  | 1.00 | 39.11  |
| ATOM | 6236 | OH2 | TIP3 | 737 | 97.536  | 64.003 | 85.787  | 1.00 | 41.08  |
| ATOM | 6237 | OH2 | TIP3 | 738 | 69.252  | 74.894 | 82.126  | 1.00 | 22.96  |
| ATOM | 6238 | OH2 | TIP3 | 739 | 71.940  | 55.321 | 80.912  | 1.00 | 34.50  |
| ATOM | 6239 | OH2 | TIP3 | 740 | 70.550  | 55.962 | 83.229  | 1.00 | 38.09  |
| ATOM | 6240 | OH2 | TIP3 | 741 | 68.530  | 50.686 | 67.504  | 1.00 | 36.49  |
| ATOM | 6241 | OH2 | TIP3 | 742 | 67.078  | 49.872 | 64.964  | 1.00 | 43.81  |
| ATOM | 6242 | OH2 | TIP3 | 743 | 79.200  | 58.771 | 55.790  | 1.00 | 36.92  |
| ATOM | 6243 | OH2 | TIP3 | 744 | 87.067  | 77.893 | 23.397  | 1.00 | 43.96  |
| ATOM | 6244 | OH2 | TIP3 | 745 | 54.640  | 58.967 | 38.719  | 1.00 | 36.98  |
| ATOM | 6245 | OH2 | TIP3 | 746 | 51.786  | 59.284 | 33.944  | 1.00 | 44.76  |
| ATOM | 6246 | OH2 | TIP3 | 747 | 90.904  | 49.068 | 36.430  | 1.00 | 163.82 |
| ATOM | 6247 | OH2 | TIP3 | 748 | 82.871  | 63.204 | 61.483  | 1.00 | 41.80  |
| ATOM | 6248 | OH2 | TIP3 | 749 | 88.761  | 50.228 | 82.920  | 1.00 | 58.55  |
| ATOM | 6249 | OH2 | TIP3 | 750 | 81.750  | 74.065 | 103.304 | 1.00 | 39.00  |

FIGURE 1 (CONT.)

|      |      |     |      |     |        |         |         |      |        |
|------|------|-----|------|-----|--------|---------|---------|------|--------|
| ATOM | 6250 | OH2 | TIP3 | 751 | 66.504 | 88.568  | 77.984  | 1.00 | 65.75  |
| ATOM | 6251 | OH2 | TIP3 | 752 | 69.412 | 89.769  | 82.897  | 1.00 | 56.13  |
| ATOM | 6252 | OH2 | TIP3 | 753 | 82.689 | 72.715  | 67.756  | 1.00 | 22.04  |
| ATOM | 6253 | OH2 | TIP3 | 754 | 93.644 | 47.147  | 67.273  | 1.00 | 54.18  |
| ATOM | 6254 | OH2 | TIP3 | 755 | 97.081 | 53.639  | 71.995  | 1.00 | 69.31  |
| ATOM | 6255 | OH2 | TIP3 | 756 | 70.064 | 87.291  | 62.433  | 1.00 | 102.37 |
| ATOM | 6256 | OH2 | TIP3 | 757 | 73.191 | 90.367  | 65.078  | 1.00 | 50.53  |
| ATOM | 6257 | OH2 | TIP3 | 758 | 67.919 | 65.829  | 34.994  | 1.00 | 46.46  |
| ATOM | 6258 | OH2 | TIP3 | 759 | 67.766 | 62.682  | 29.909  | 1.00 | 48.04  |
| ATOM | 6259 | OH2 | TIP3 | 760 | 67.898 | 67.872  | 33.364  | 1.00 | 55.10  |
| ATOM | 6260 | OH2 | TIP3 | 761 | 75.277 | 82.599  | 61.330  | 1.00 | 58.80  |
| ATOM | 6261 | OH2 | TIP3 | 762 | 74.827 | 82.595  | 58.575  | 1.00 | 49.19  |
| ATOM | 6262 | OH2 | TIP3 | 763 | 83.123 | 64.992  | 45.218  | 1.00 | 29.88  |
| ATOM | 6263 | OH2 | TIP3 | 764 | 84.728 | 65.820  | 66.470  | 1.00 | 45.69  |
| ATOM | 6264 | OH2 | TIP3 | 765 | 85.961 | 70.489  | 71.473  | 1.00 | 38.35  |
| ATOM | 6265 | OH2 | TIP3 | 766 | 87.324 | 68.224  | 72.271  | 1.00 | 28.55  |
| ATOM | 6266 | OH2 | TIP3 | 767 | 84.928 | 69.467  | 73.731  | 1.00 | 44.55  |
| ATOM | 6267 | OH2 | TIP3 | 768 | 76.765 | 62.520  | 103.736 | 1.00 | 58.67  |
| ATOM | 6268 | OH2 | TIP3 | 769 | 84.140 | 39.796  | 28.646  | 1.00 | 45.66  |
| ATOM | 6269 | OH2 | TIP3 | 770 | 83.628 | 41.922  | 32.632  | 1.00 | 43.68  |
| ATOM | 6270 | OH2 | TIP3 | 771 | 82.432 | 41.152  | 35.014  | 1.00 | 41.03  |
| ATOM | 6271 | OH2 | TIP3 | 772 | 85.785 | 40.516  | 31.870  | 1.00 | 77.32  |
| ATOM | 6272 | OH2 | TIP3 | 773 | 61.289 | 85.672  | 83.306  | 1.00 | 52.50  |
| ATOM | 6273 | OH2 | TIP3 | 774 | 80.035 | 101.956 | 82.899  | 1.00 | 37.06  |
| ATOM | 6274 | OH2 | TIP3 | 775 | 63.097 | 79.370  | 68.380  | 1.00 | 24.13  |
| ATOM | 6275 | OH2 | TIP3 | 776 | 88.040 | 87.256  | 70.554  | 1.00 | 40.73  |
| ATOM | 6276 | OH2 | TIP3 | 777 | 66.901 | 59.286  | 59.258  | 1.00 | 43.62  |
| ATOM | 6277 | OH2 | TIP3 | 778 | 81.864 | 74.462  | 75.134  | 1.00 | 36.80  |
| ATOM | 6278 | OH2 | TIP3 | 779 | 83.881 | 83.471  | 99.167  | 1.00 | 44.32  |
| ATOM | 6279 | OH2 | TIP3 | 780 | 83.457 | 80.677  | 98.481  | 1.00 | 44.09  |
| ATOM | 6280 | OH2 | TIP3 | 781 | 82.376 | 85.551  | 101.068 | 1.00 | 37.49  |
| ATOM | 6281 | OH2 | TIP3 | 782 | 75.550 | 74.768  | 98.408  | 1.00 | 52.97  |
| ATOM | 6282 | OH2 | TIP3 | 783 | 73.955 | 78.953  | 101.355 | 1.00 | 57.37  |
| ATOM | 6283 | OH2 | TIP3 | 784 | 80.713 | 64.405  | 109.404 | 1.00 | 44.25  |
| ATOM | 6284 | OH2 | TIP3 | 785 | 58.907 | 87.813  | 87.475  | 1.00 | 61.21  |
| ATOM | 6285 | OH2 | TIP3 | 786 | 80.267 | 61.506  | 96.956  | 1.00 | 36.10  |
| ATOM | 6286 | OH2 | TIP3 | 787 | 84.222 | 58.111  | 62.183  | 1.00 | 70.74  |
| ATOM | 6287 | OH2 | TIP3 | 788 | 83.160 | 57.267  | 58.302  | 1.00 | 52.72  |
| ATOM | 6288 | OH2 | TIP3 | 789 | 66.464 | 47.762  | 96.657  | 1.00 | 59.25  |
| ATOM | 6289 | OH2 | TIP3 | 790 | 69.394 | 52.614  | 90.763  | 1.00 | 48.67  |
| ATOM | 6290 | OH2 | TIP3 | 791 | 92.257 | 73.130  | 19.969  | 1.00 | 51.24  |
| ATOM | 6291 | OH2 | TIP3 | 792 | 99.638 | 61.766  | 45.543  | 1.00 | 54.79  |
| ATOM | 6292 | OH2 | TIP3 | 793 | 97.433 | 64.794  | 49.071  | 1.00 | 47.02  |
| ATOM | 6293 | OH2 | TIP3 | 794 | 77.710 | 52.845  | 32.368  | 1.00 | 35.15  |
| ATOM | 6294 | OH2 | TIP3 | 795 | 69.444 | 52.278  | 37.349  | 1.00 | 59.52  |
| ATOM | 6295 | OH2 | TIP3 | 796 | 68.211 | 49.099  | 26.477  | 1.00 | 47.09  |
| ATOM | 6296 | OH2 | TIP3 | 797 | 65.300 | 58.001  | 47.307  | 1.00 | 45.39  |
| ATOM | 6297 | OH2 | TIP3 | 798 | 67.739 | 54.960  | 47.317  | 1.00 | 52.04  |
| ATOM | 6298 | OH2 | TIP3 | 799 | 65.578 | 50.677  | 47.117  | 1.00 | 40.40  |
| ATOM | 6299 | OH2 | TIP3 | 800 | 70.910 | 67.580  | 52.751  | 1.00 | 35.66  |
| ATOM | 6300 | OH2 | TIP3 | 801 | 70.015 | 69.737  | 50.764  | 1.00 | 27.41  |
| ATOM | 6301 | OH2 | TIP3 | 802 | 80.334 | 70.409  | 42.183  | 1.00 | 97.77  |
| ATOM | 6302 | OH2 | TIP3 | 803 | 64.245 | 76.692  | 48.798  | 1.00 | 16.97  |
| ATOM | 6303 | OH2 | TIP3 | 804 | 65.457 | 76.921  | 51.491  | 1.00 | 31.17  |

FIGURE 2





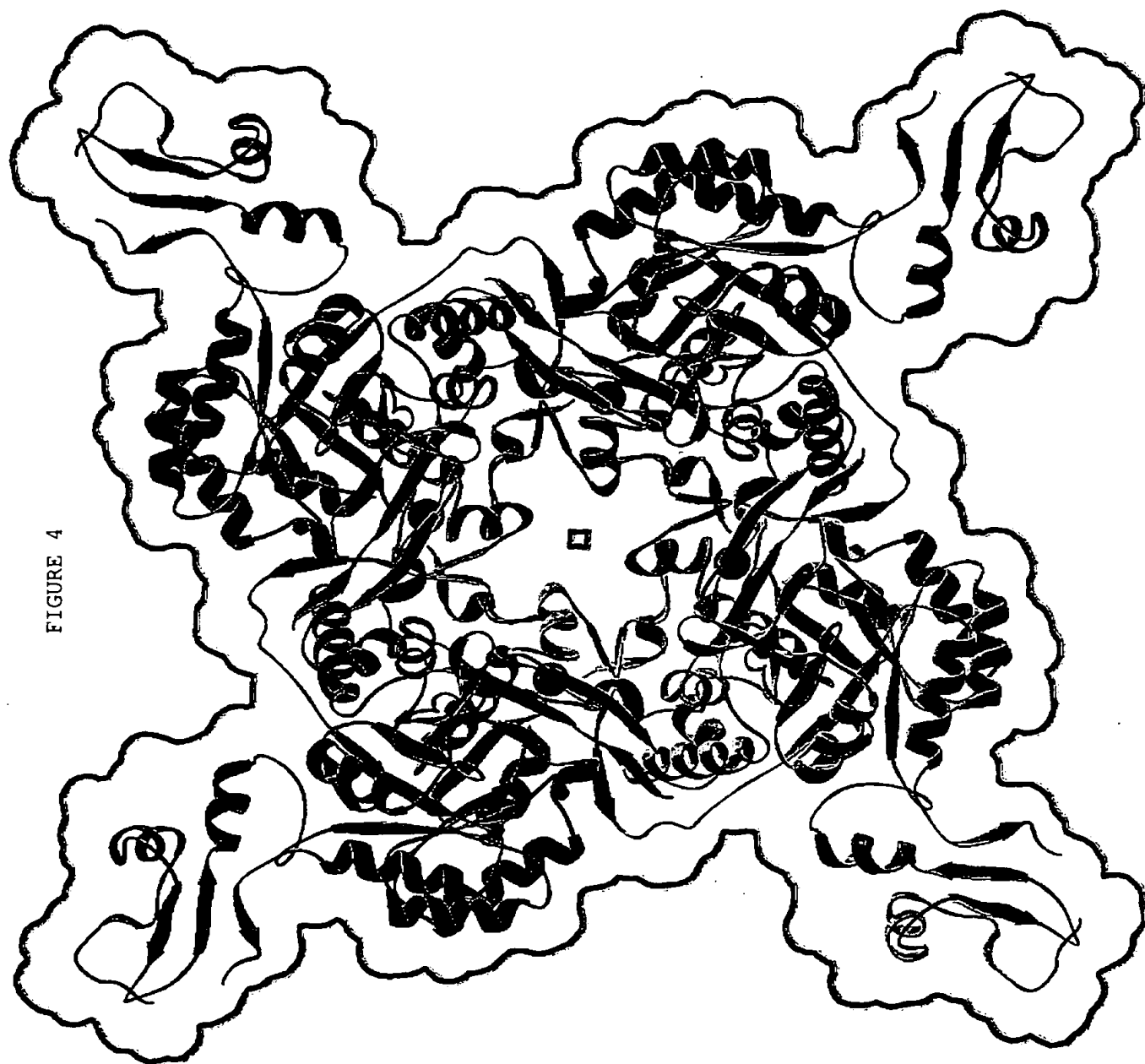


FIGURE 4



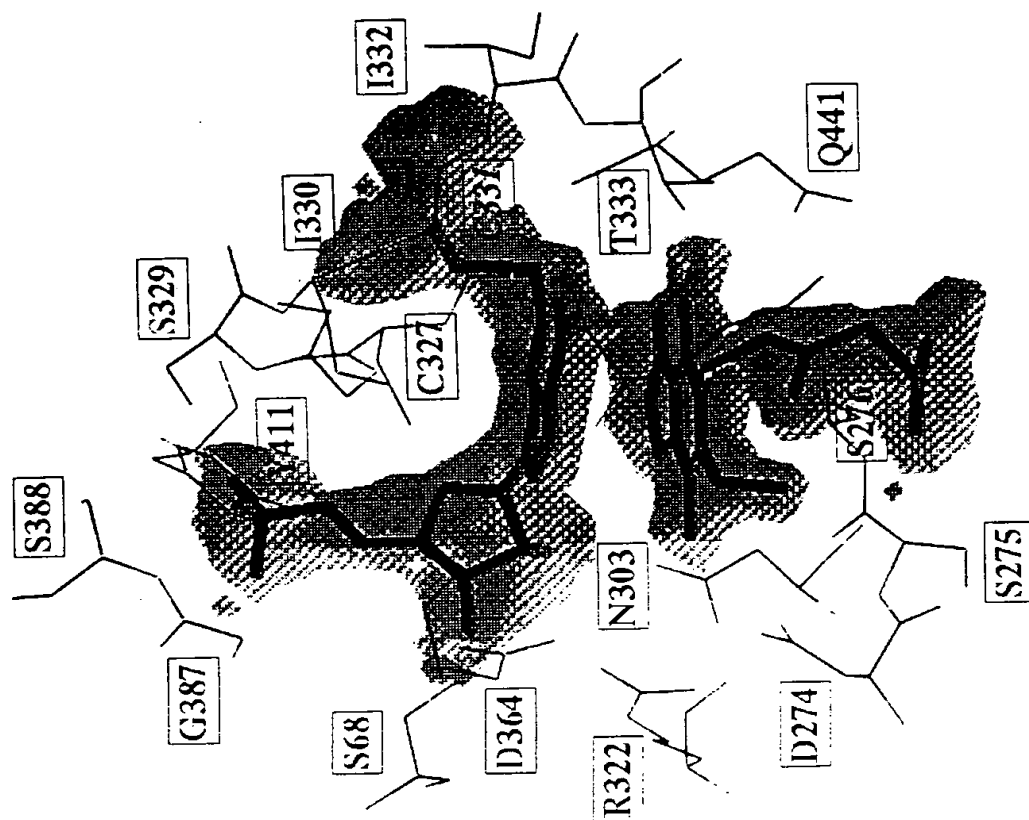


FIGURE 5

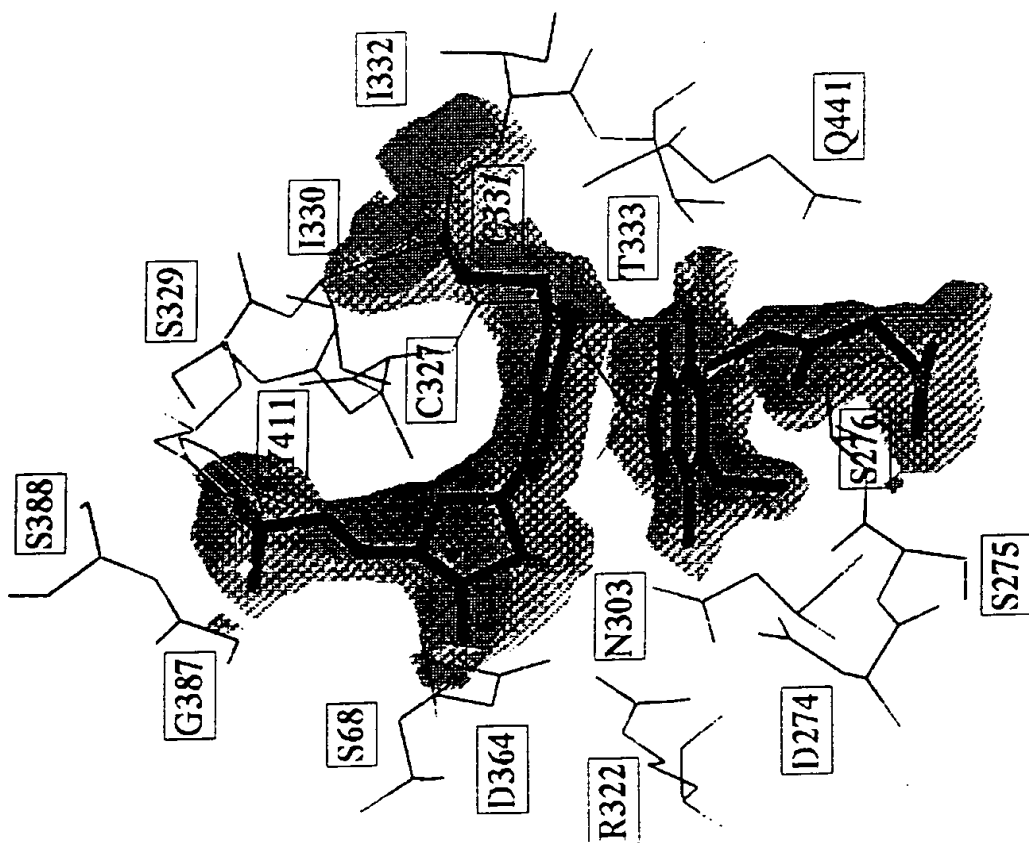


FIGURE 6  
XMP\* interactions

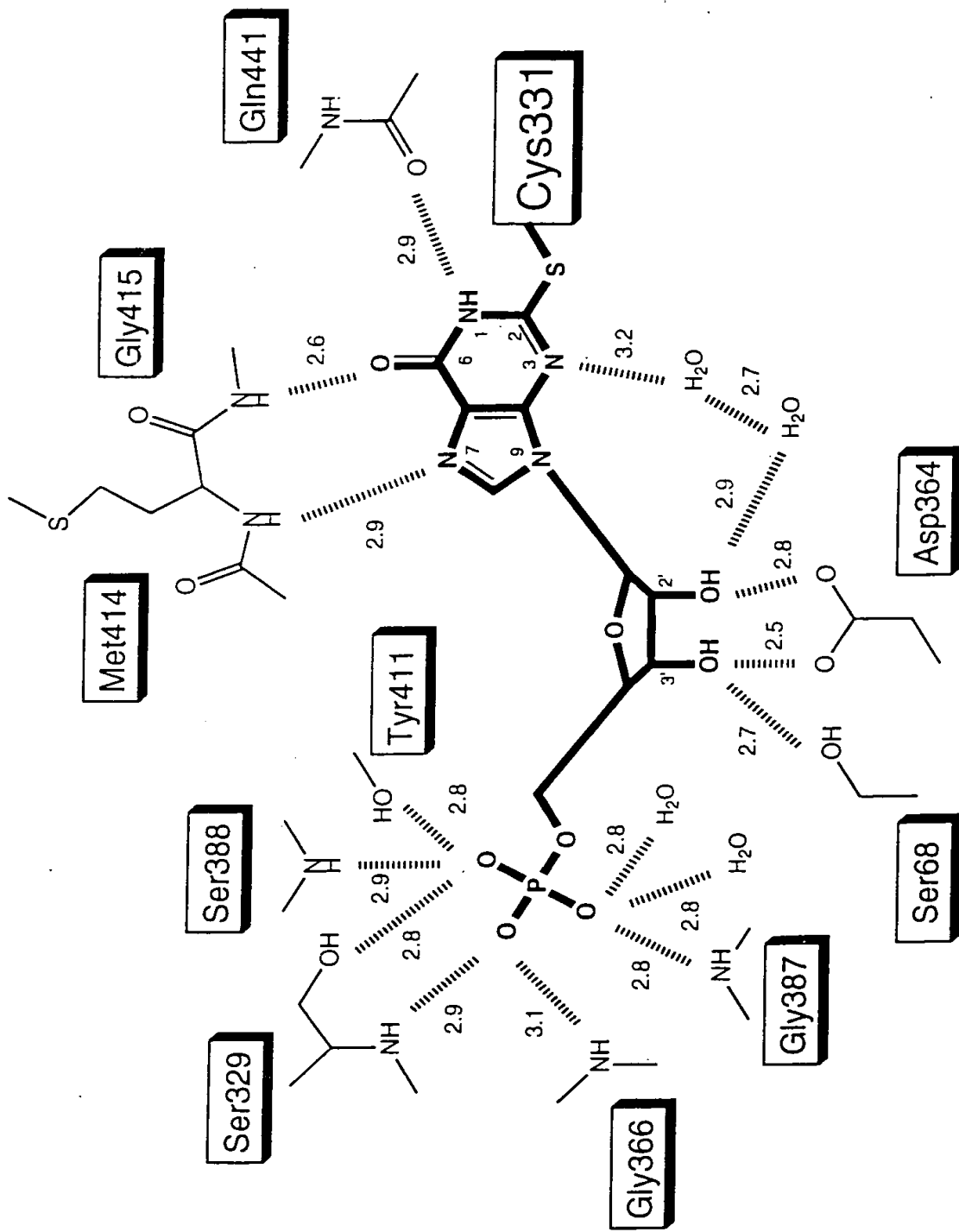


FIGURE 7

# MPA interactions

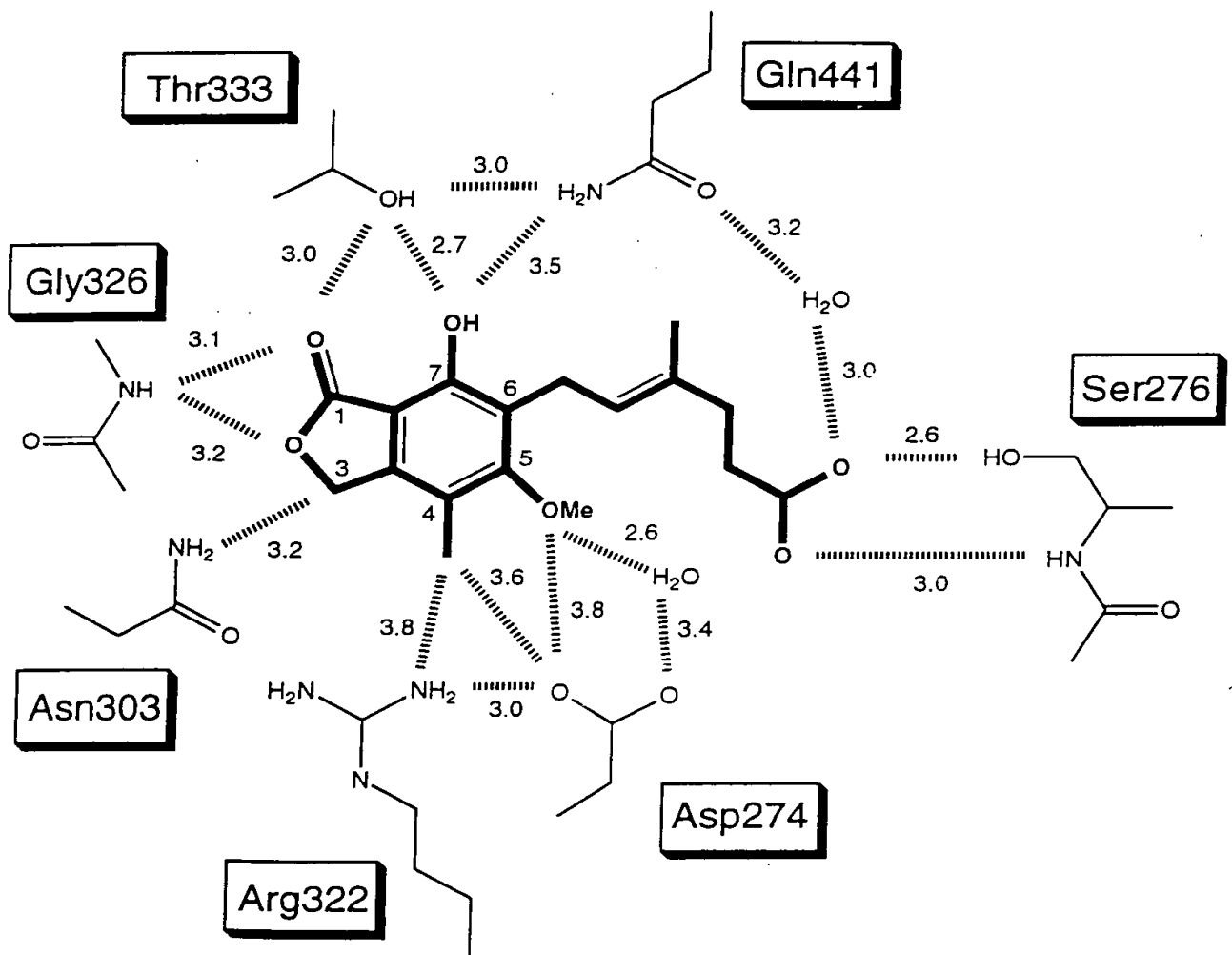


FIGURE 8

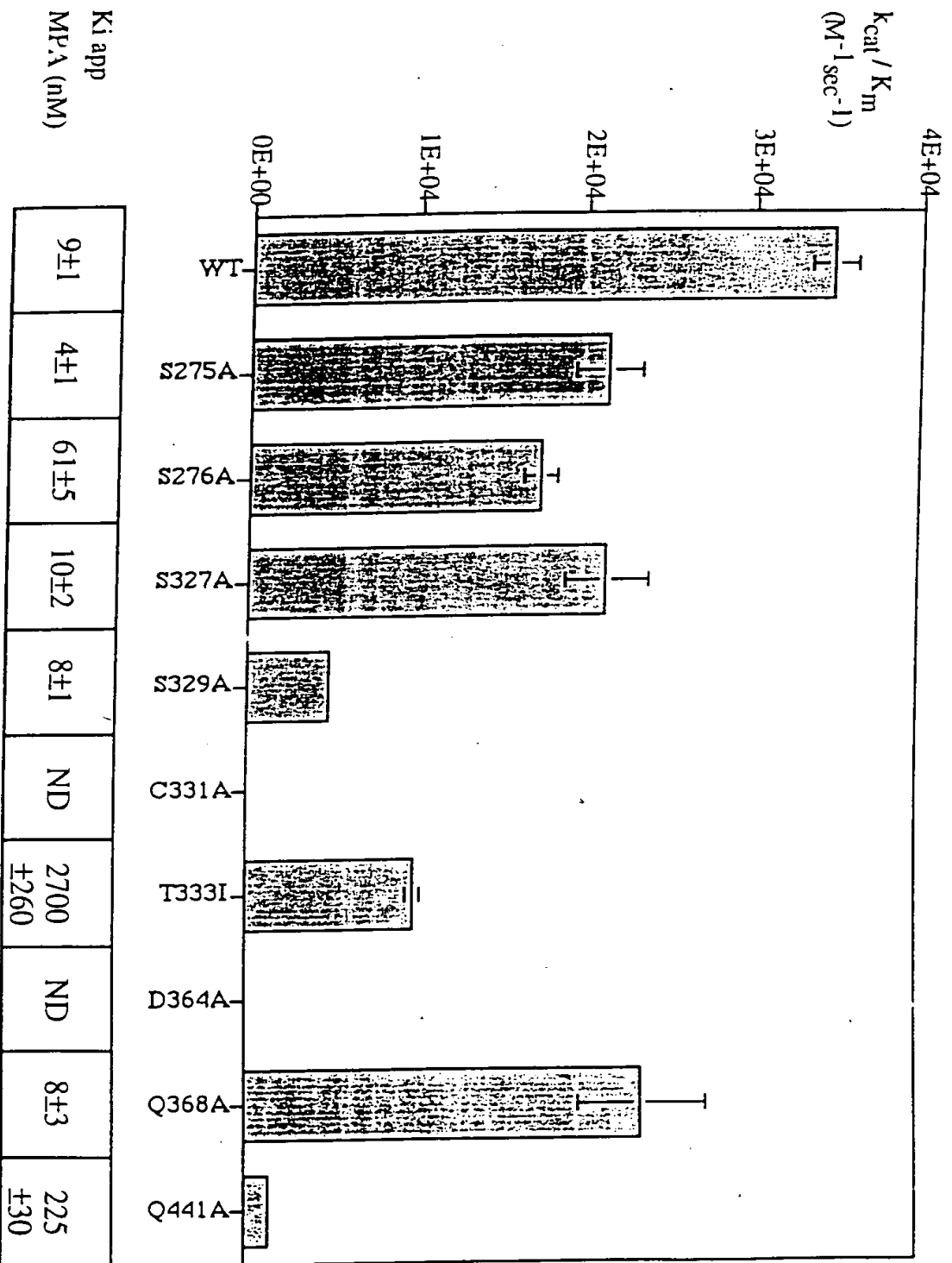


FIGURE 9

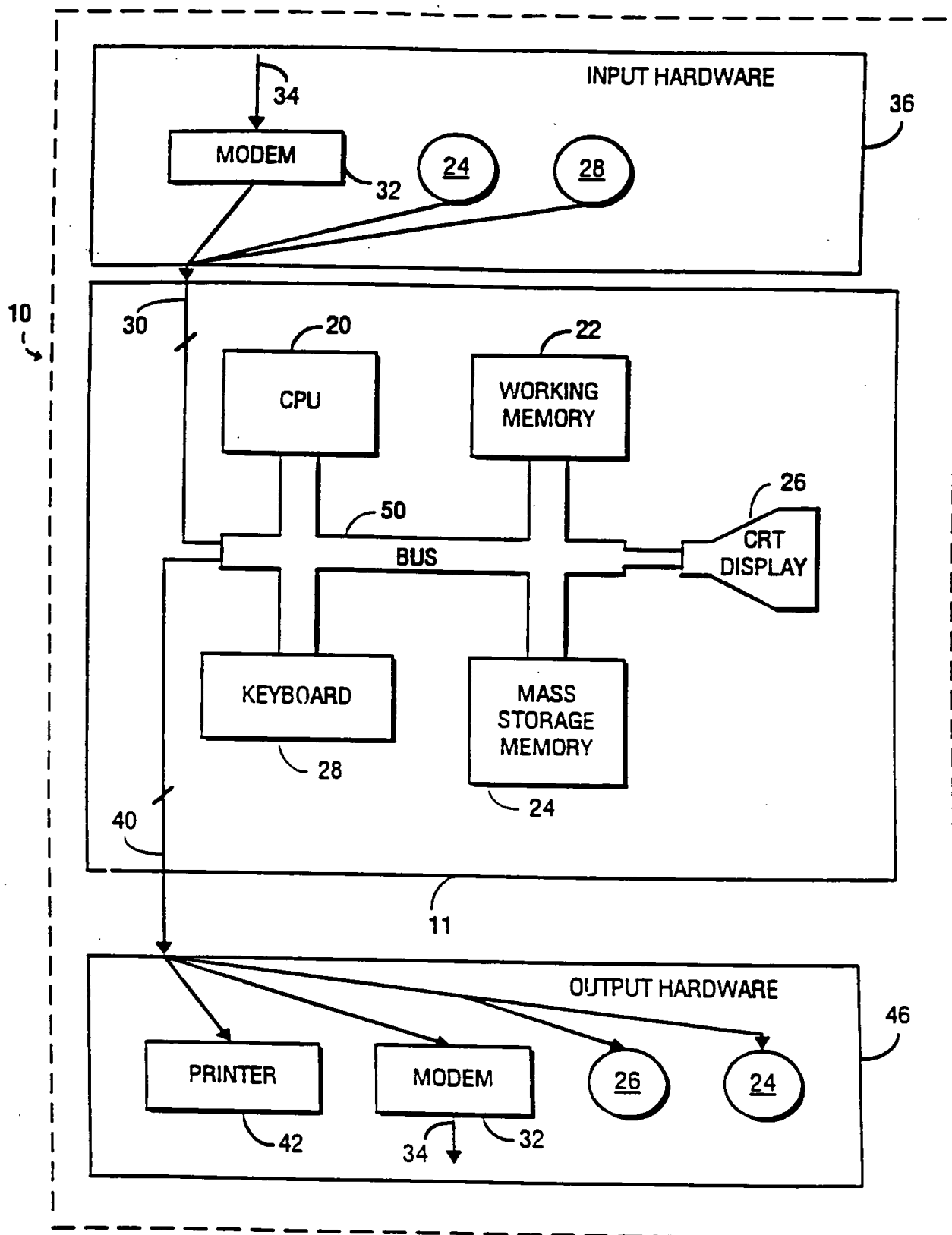


FIGURE 10

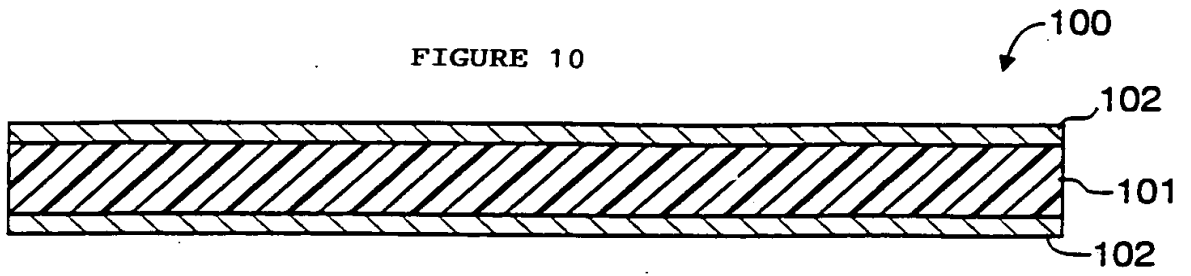


FIGURE 11

